

# Challenges in Infrared Spectroscopy Based Non-Targeted Analysis

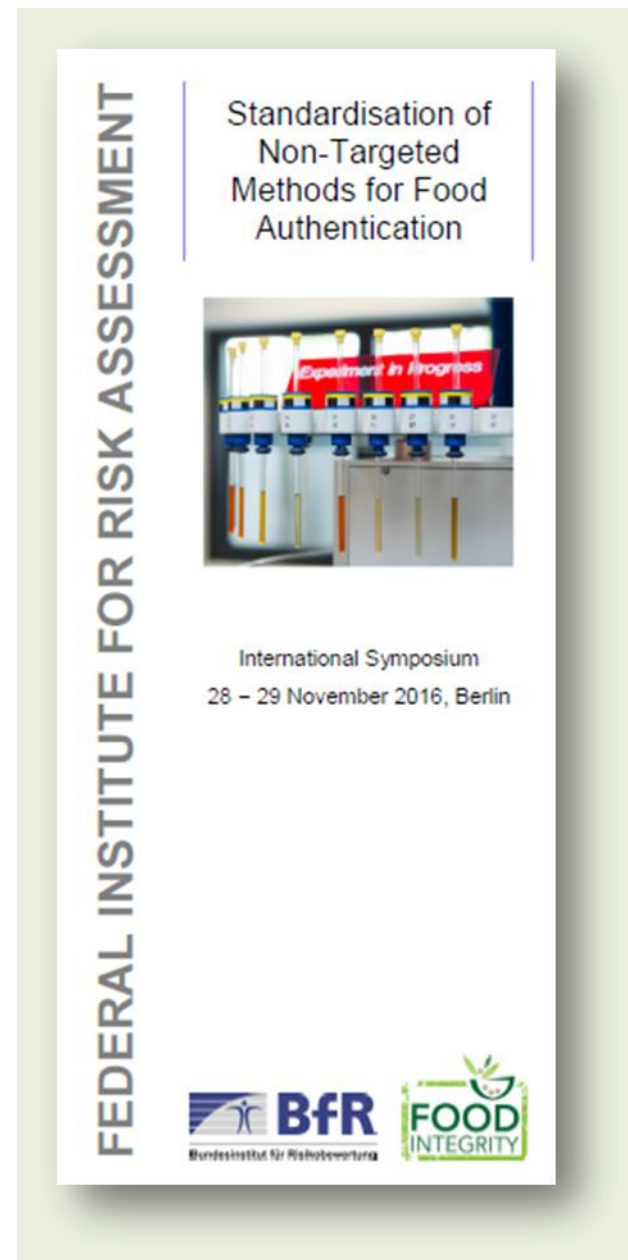
**Vincent Baeten**

**Juan A. Fernández Pierna  
Clément Grelet (U14)  
Frédéric Dehareng (U14)  
Pierre Dardenne (D4)**

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## Regional public body

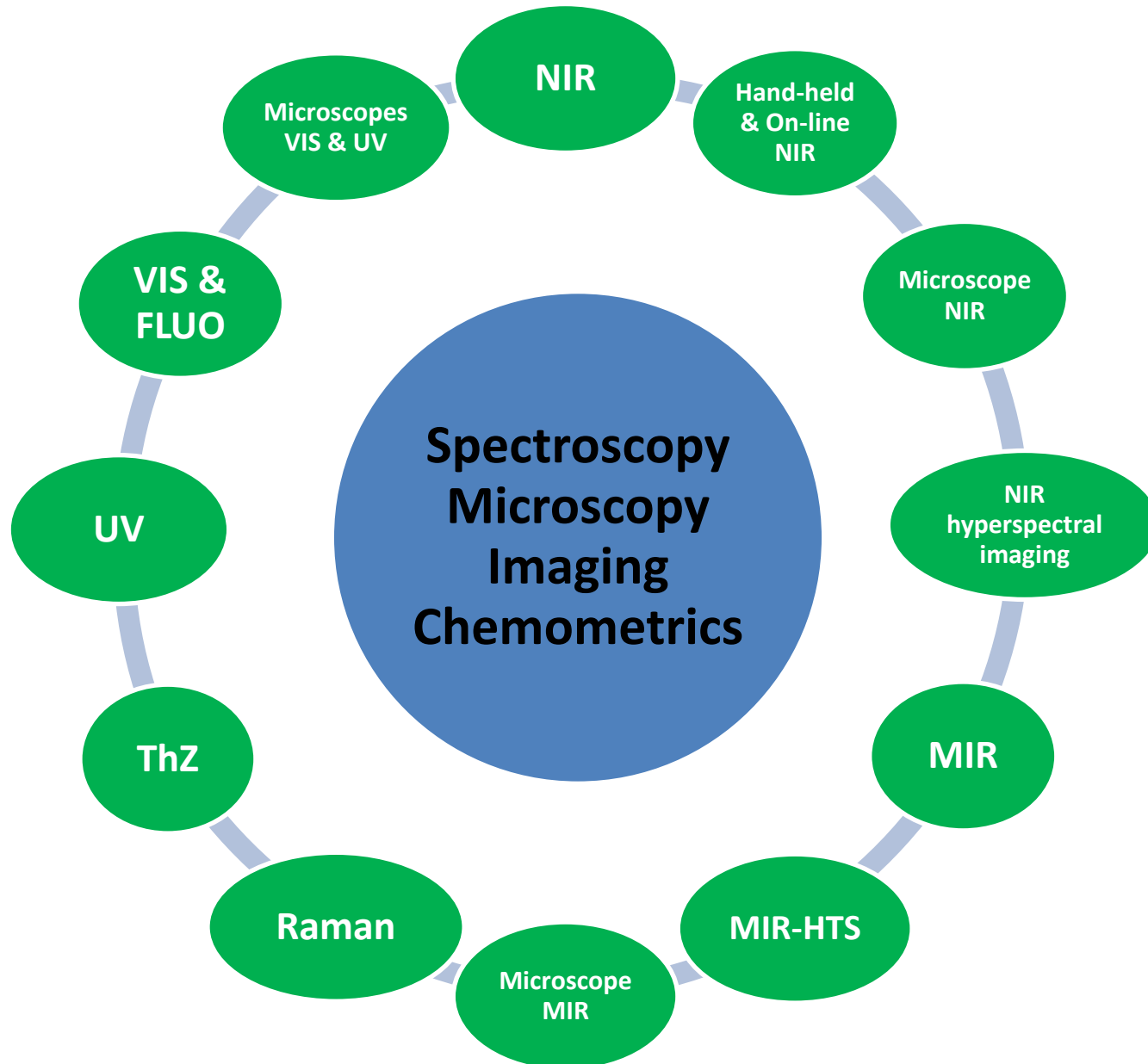
To carry out fundamental and applied agricultural research programmes



## 4 Research Departments

1. Life sciences
2. Production and sectors
3. Agriculture and natural environment
- 4. Valorisation of agricultural products (Pierre Dardenne)**

**- Food and Feed Quality Unit (Vincent Baeten)**



# Food and Feed Quality Unit



**Our goal :**  
Development of analytical solutions for farmers, factories, retailers, distributors, control bodies and consumers

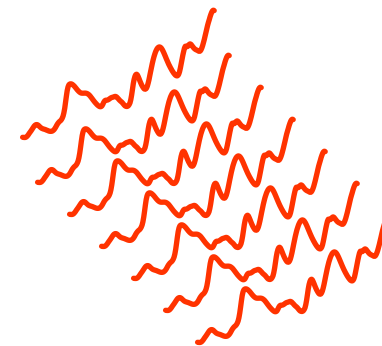
# CHALLENGE



Related tags: IDF, Dairy, Milk, Adulteration

<http://www.afia.org/>

# NIRS/Feed --- a mature technique in continuous progression

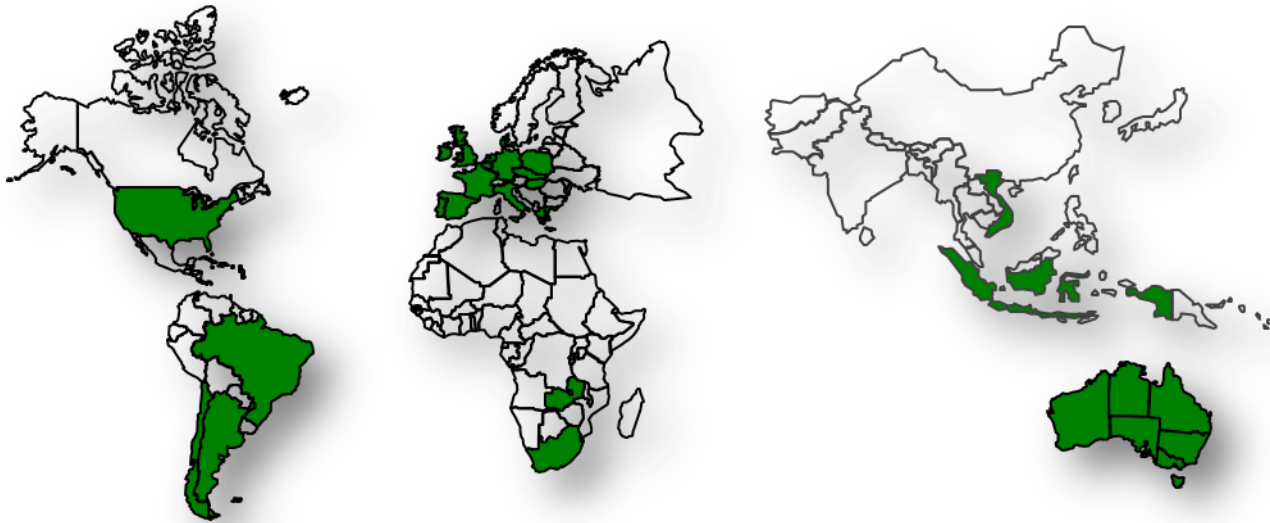


**NIRS**  
(Near Infrared Spectroscopy)

**NIRS contribution to the FeedOmics**

# The advantages of instrument networks

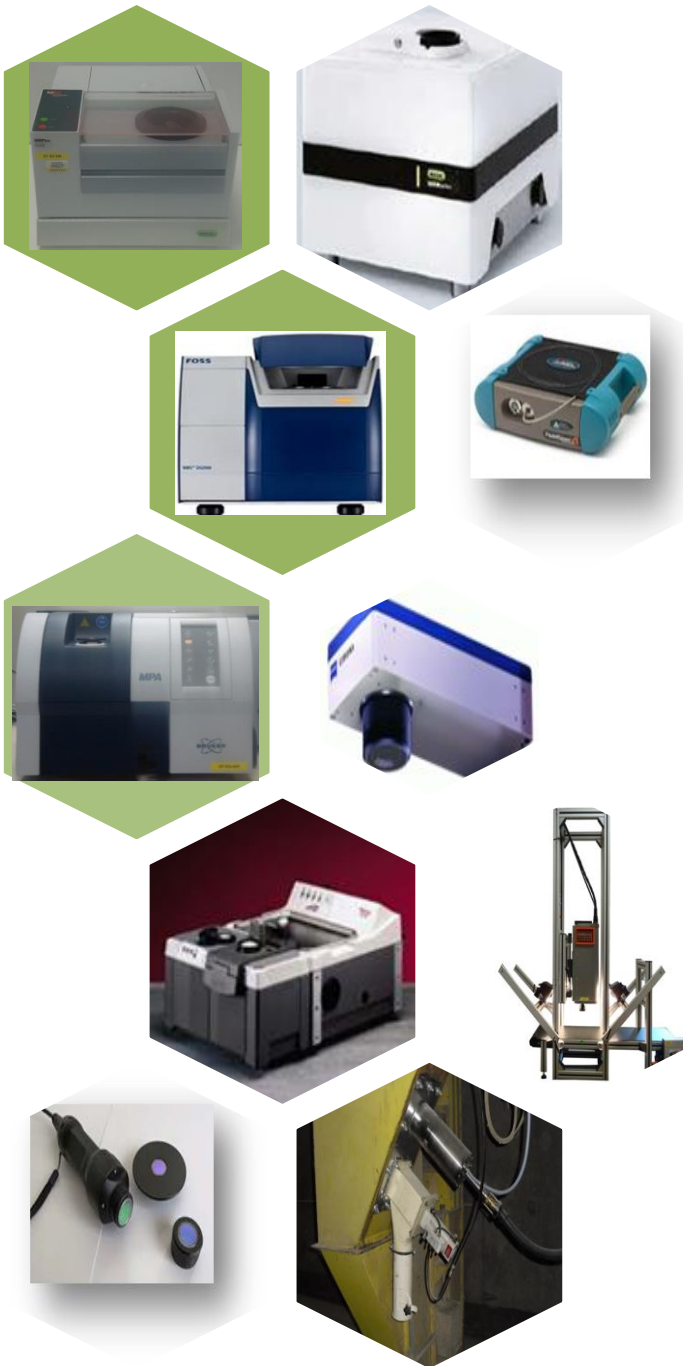
Use of IR and Network of instruments: a reality!  
Provimi : > 240 instruments



- Prediction of:
  - Dry matter
  - Organic matter digestibility
  - Crude protein
  - Cellulose
- Detection of contaminants

# What are the challenges?

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

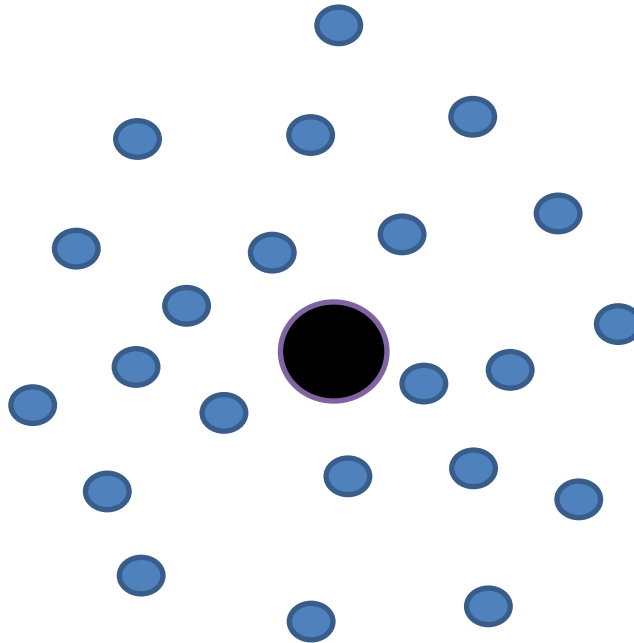




# Standardisation of instruments : How it works?

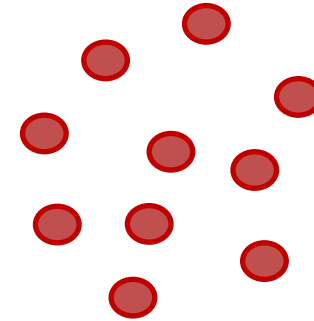


Brand C

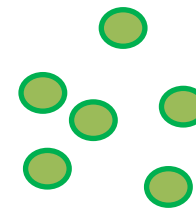


# Standardisation of instruments : How it works?

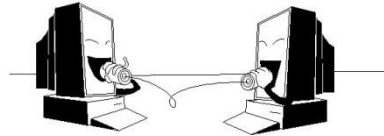
Brand B



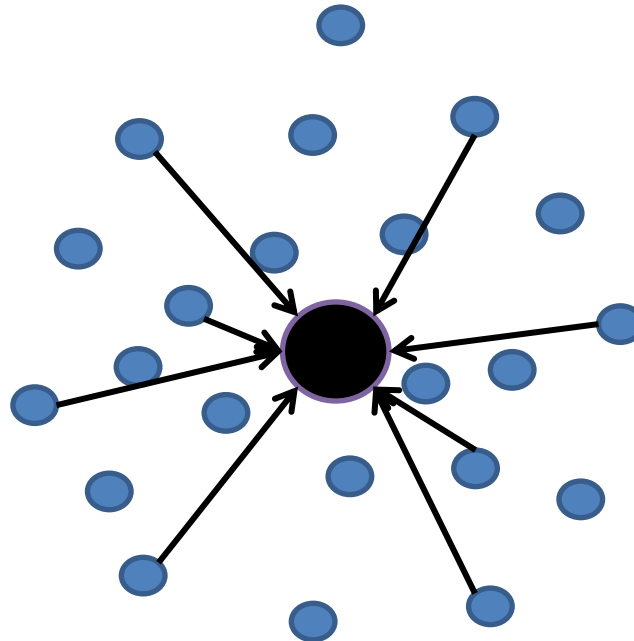
Brand A



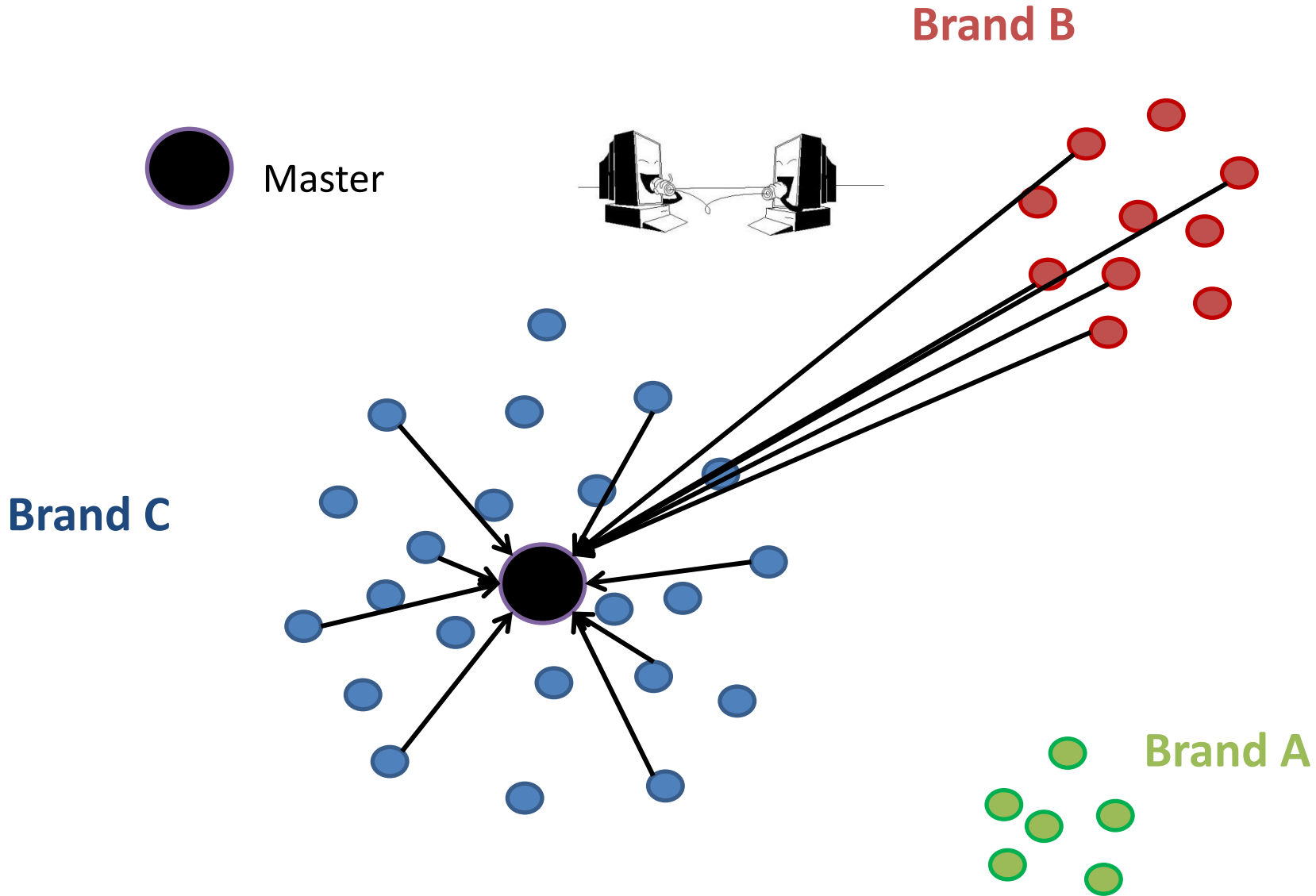
Master



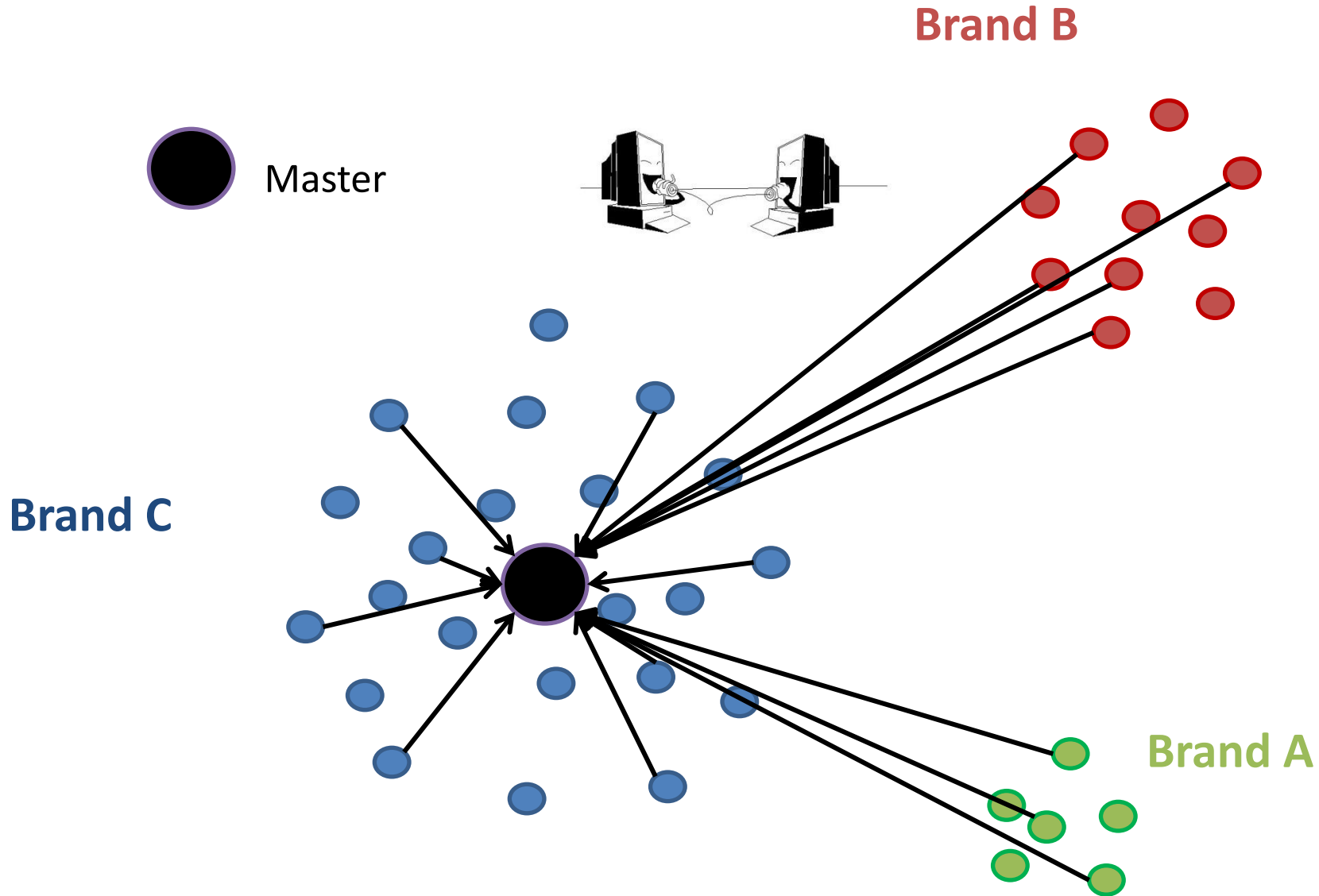
Brand C



# Standardisation of instruments : How it works?



# Standardisation of instruments : How it works?



# Standardisation : a procedure to assess that spectrometers from a network speak the same language



<http://flixtranslations.com/>

Standardised instruments for creation of equations

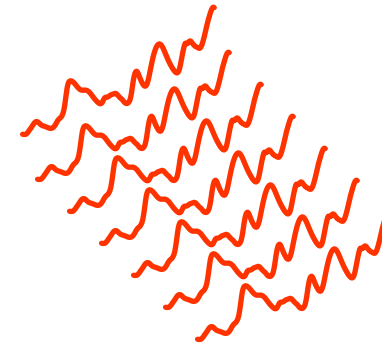
Standardised instruments for use of equations

Standardised databases for untarget analysis strategies

# MIR/Food --- a mature technique in continuous progression



Related tags: IDF, Dairy, Milk, Adulteration



**MIR**  
(Mid Infrared Spectroscopy)

**MIR contribution to the FoodOmics**

# MIR / Milk



→ Create common database

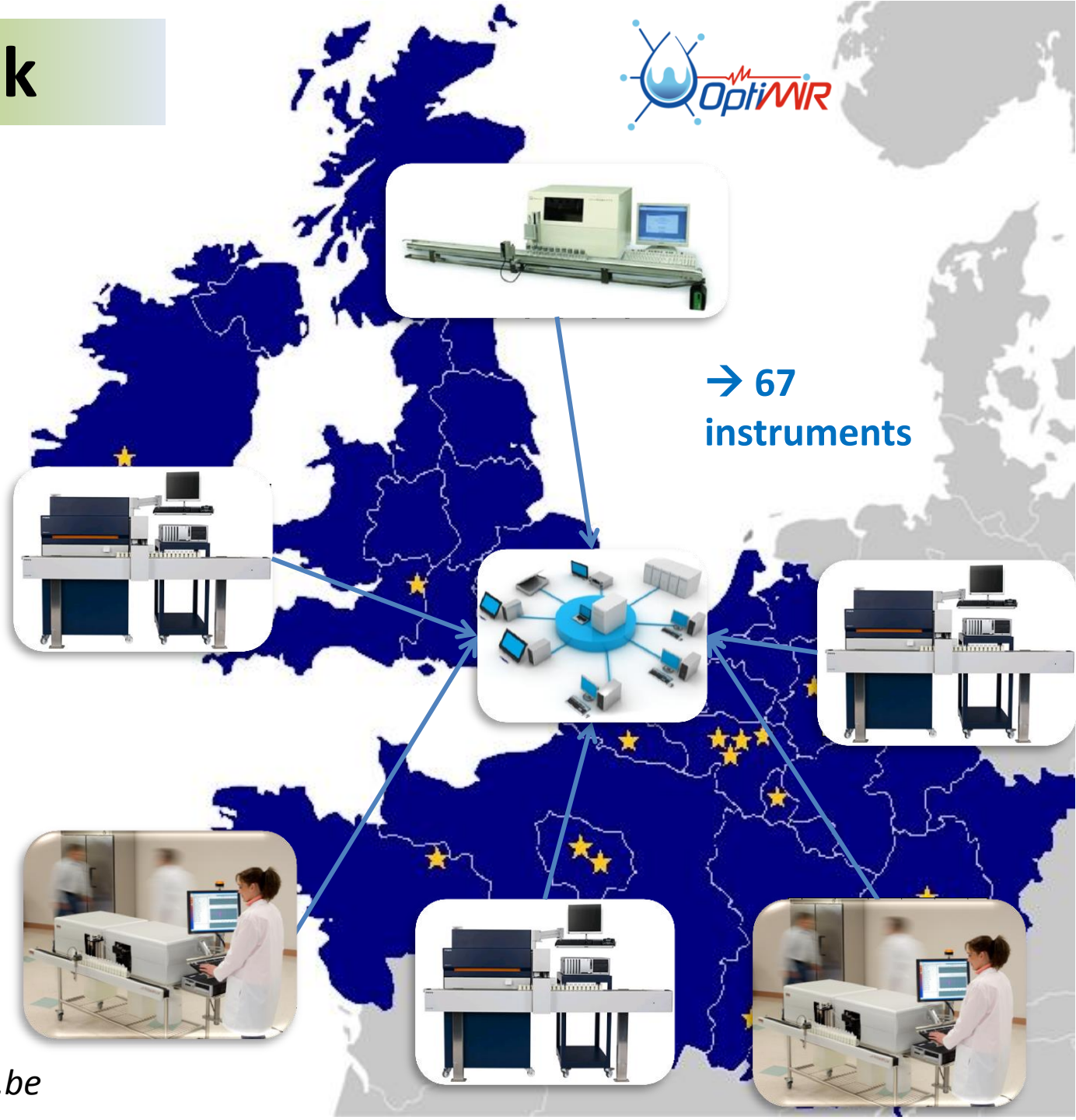
→ Create common MIR models

→ Use common MIR models

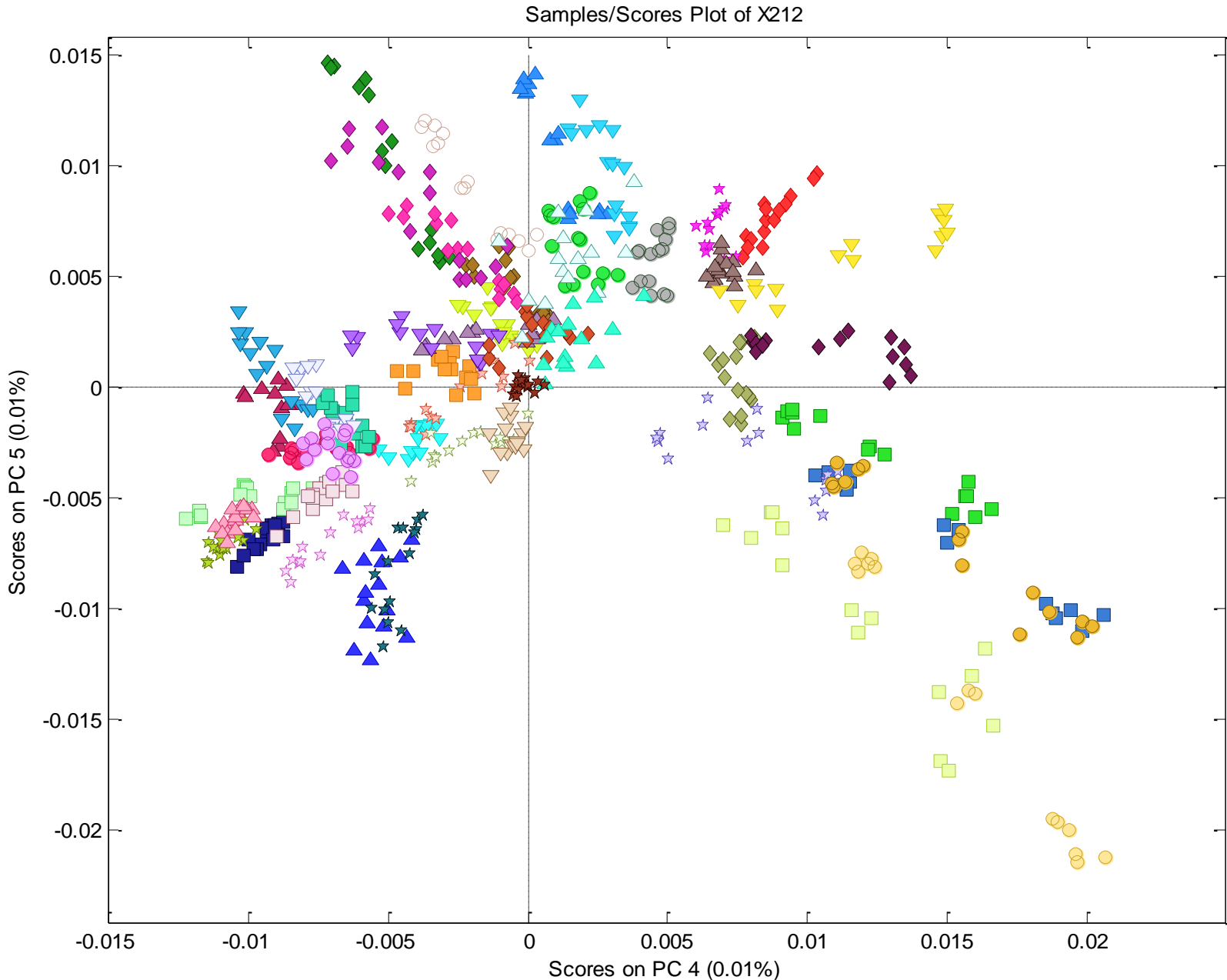
→ Have the same predictions within the network



Frédéric Dehareng  
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# MIR / Milk : variability of instruments response



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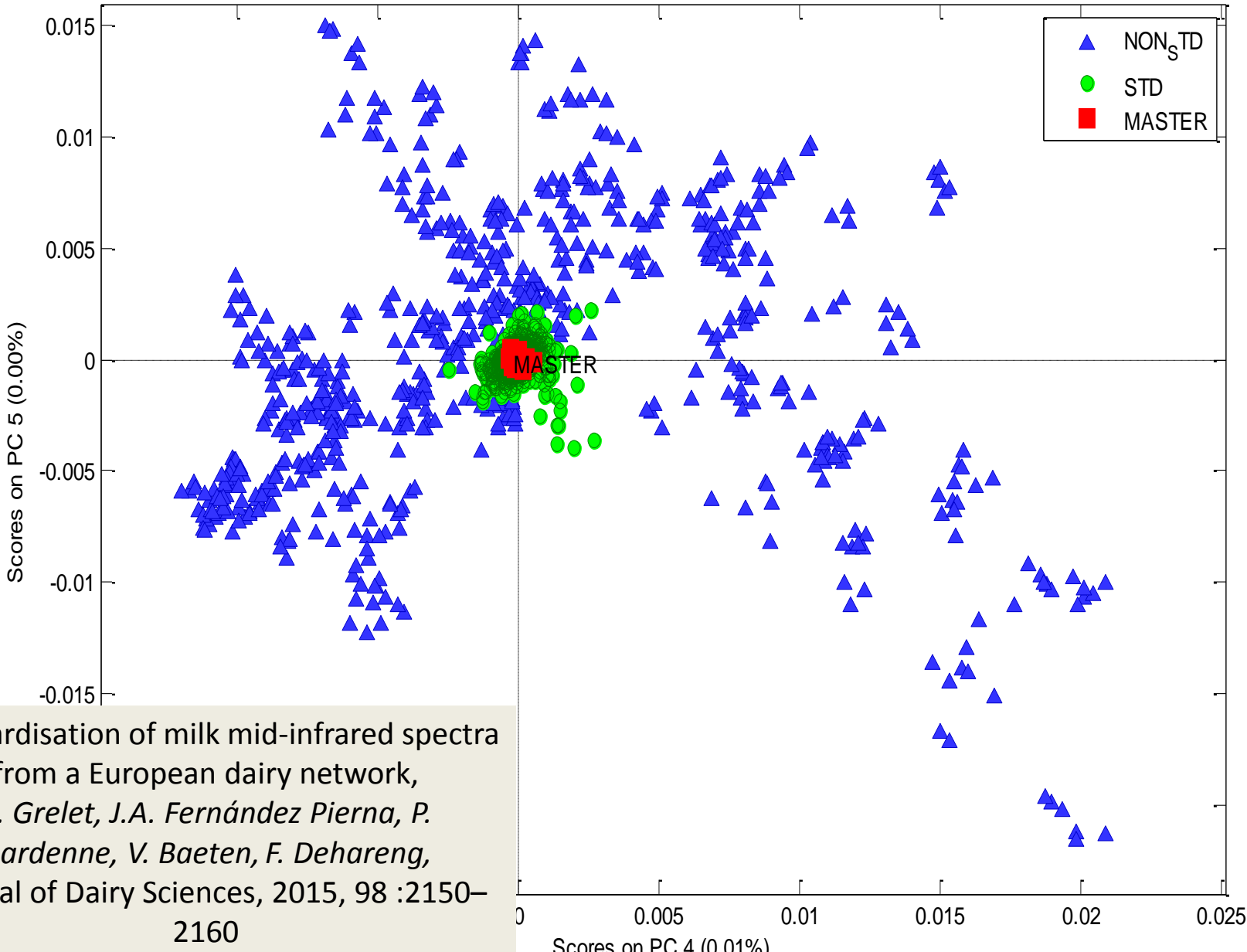




# MIR / Milk : variability of instruments response



Samples/Scores Plot of X212



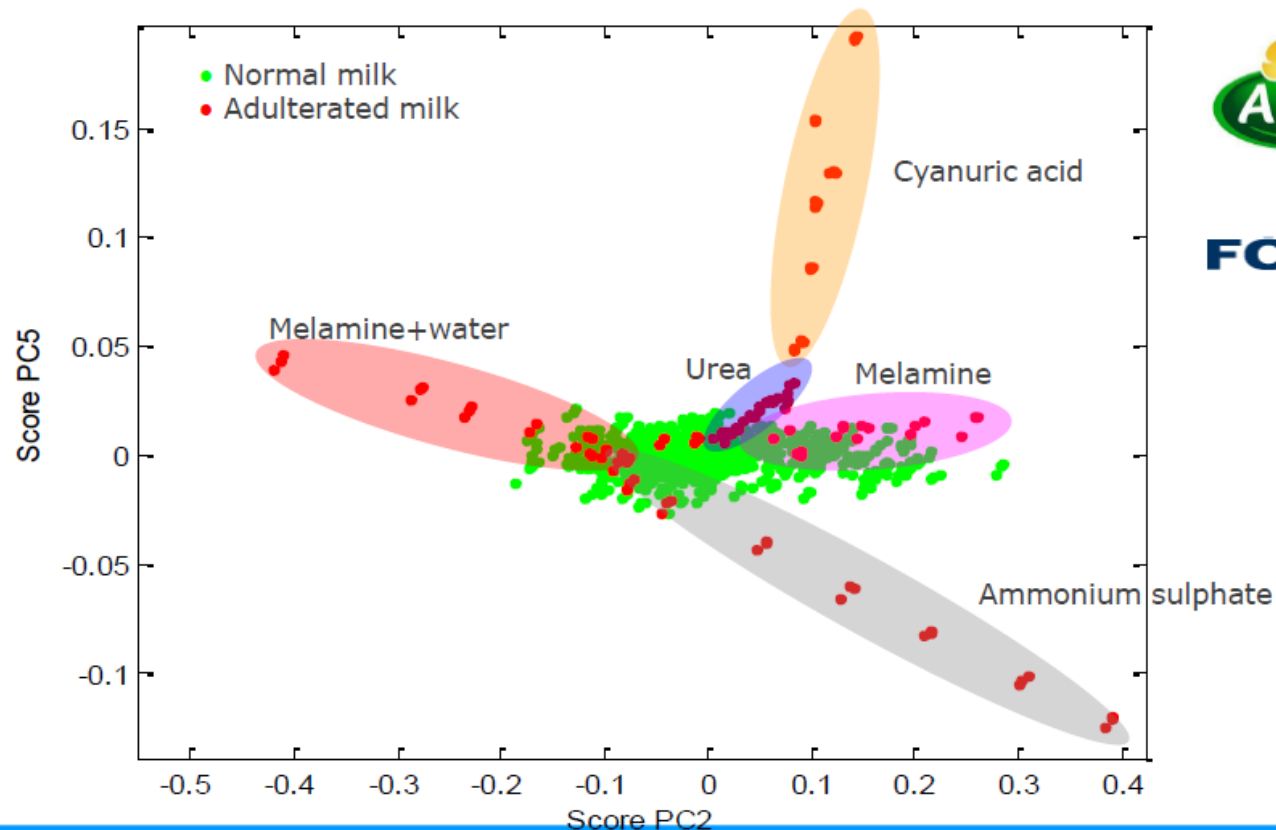
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Standardisation of milk mid-infrared spectra from a European dairy network, C. Grelet, J.A. Fernández Pierna, P. Dardenne, V. Baeten, F. Dehareng, Journal of Dairy Sciences, 2015, 98 :2150–2160



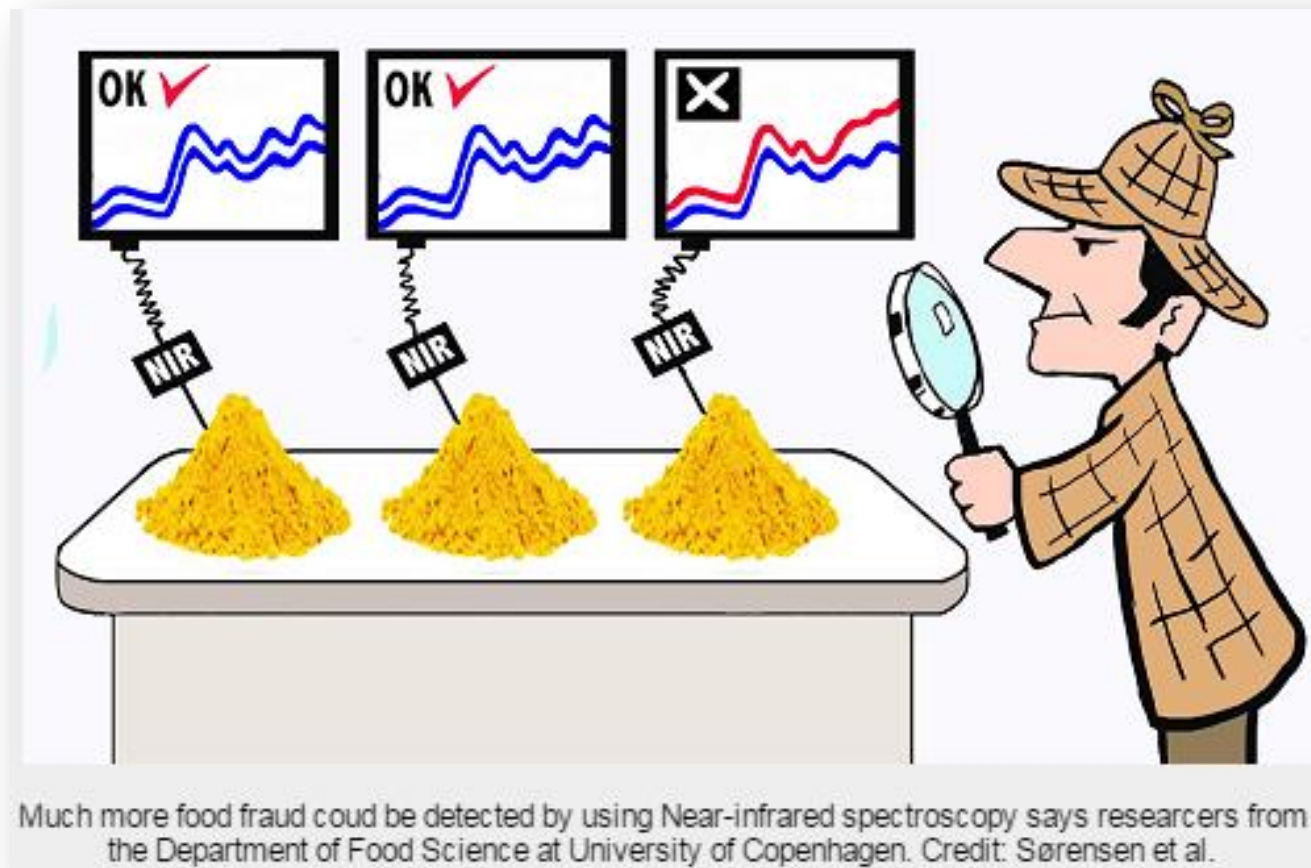
# Melamine crisis outputs

## Mid IR on liquid milk – qualitative models



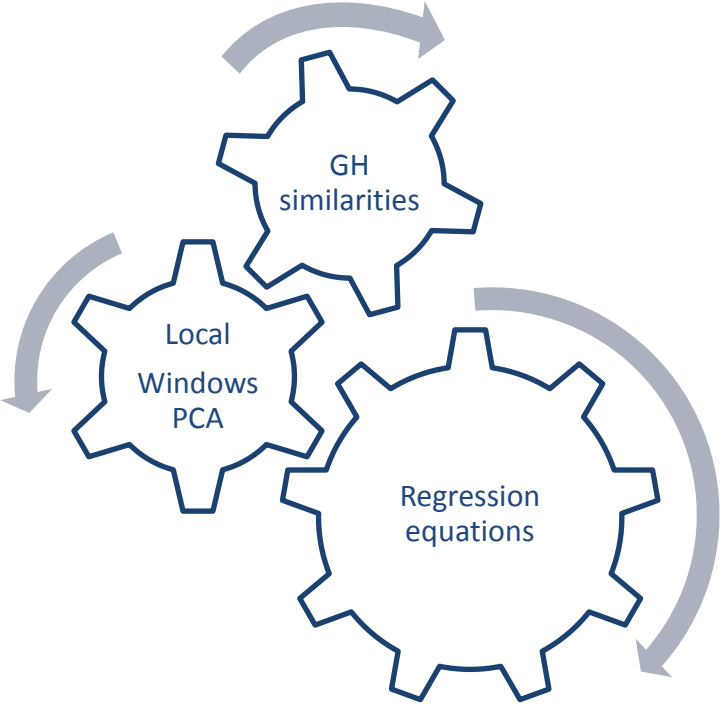
Holroyd (2011). *The role of NIR spectroscopy in maintaining food integrity. ICNIRS conference 2011, Cape Town, South Africa.*

# IR techniques - screening methods



lavs Martin Sørensen et al, *The use of rapid spectroscopic screening methods to detect adulteration of food raw materials and ingredients*, *Current Opinion in Food Science* (2016). [DOI: 10.1016/j.cofs.2016.08.001](https://doi.org/10.1016/j.cofs.2016.08.001)

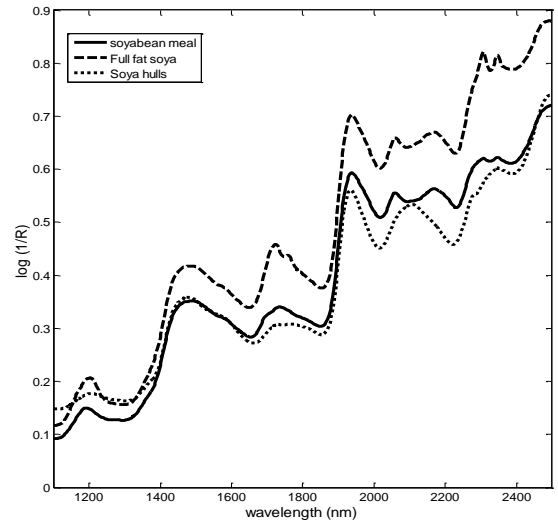
# Our "3 steps" strategy



Vincent Baeten, Philippe Vermeulen, Juan Antonio Fernández Piema and Pierre Dardenne  
Wallon Agricultural Research Centre (CRA-W), Belgium

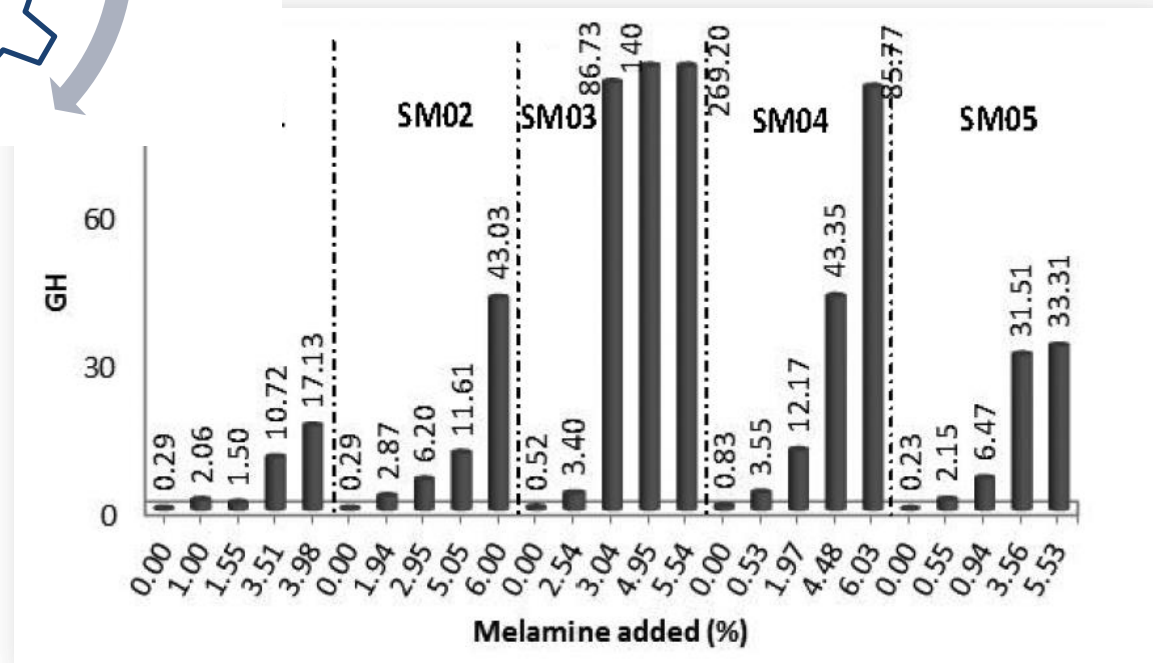
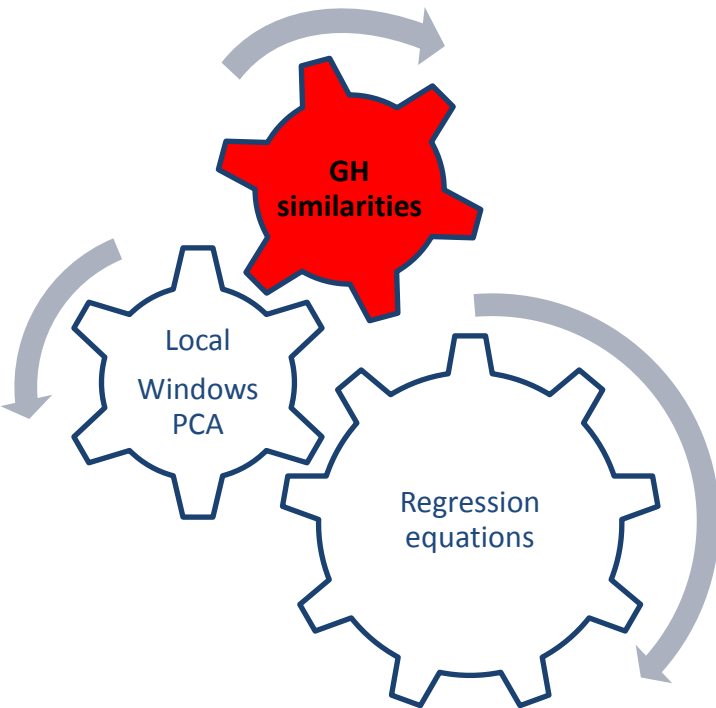
From targeted to untargeted detection of contaminants and foreign bodies in food and feed using NIR spectroscopy

**Several criteria**



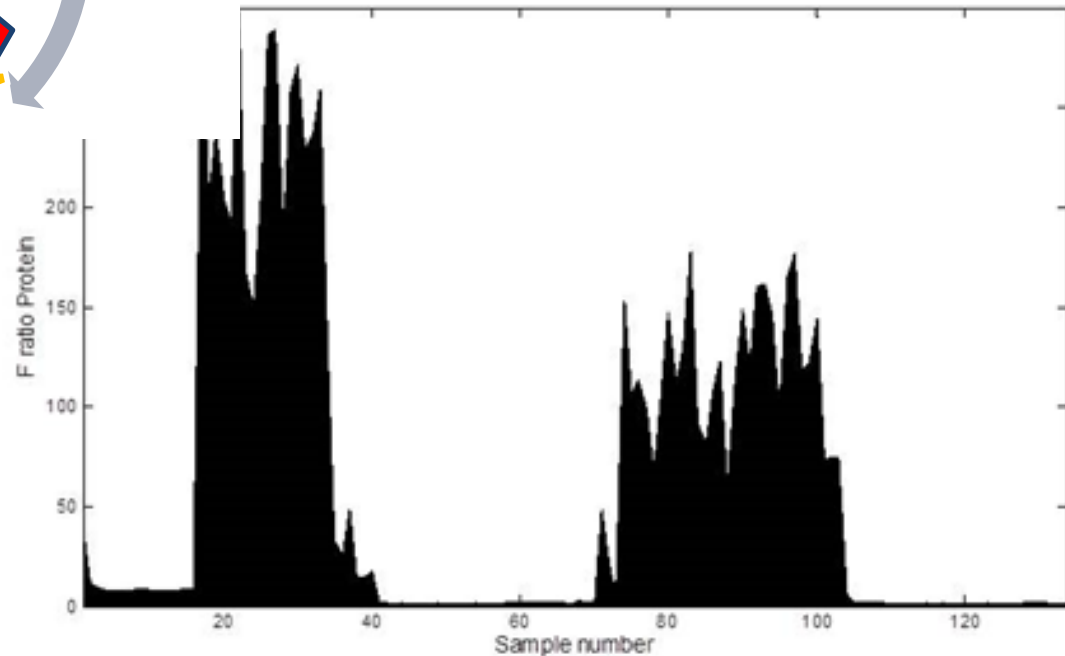
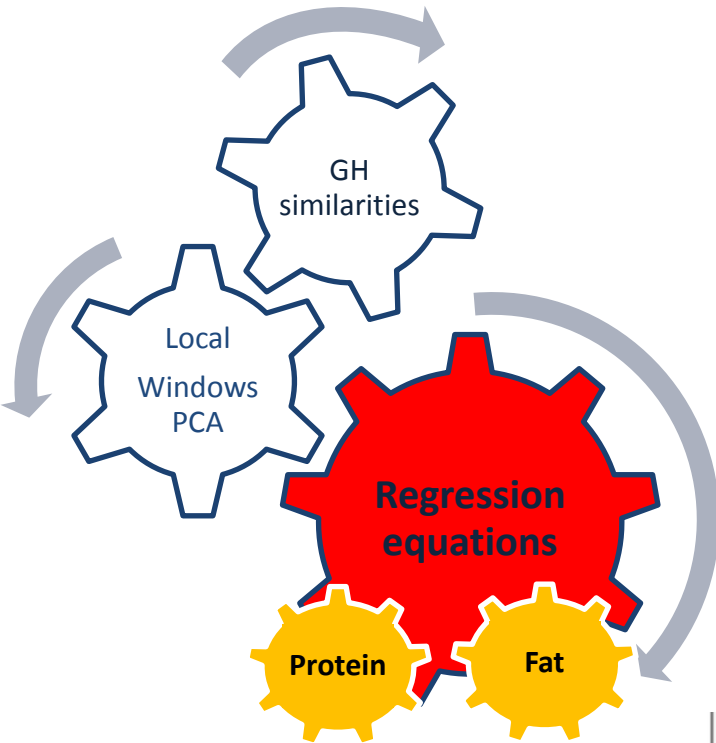
# Our "3 steps" strategy – similarities

Abbas O., Lecler B., Dardenne P. and Baeten V. (2013) **Detection of melamine in feed ingredients by near infrared spectroscopy and chemometrics.** *Journal of Near Infrared Spectroscopy*, 21(3), 183-194.



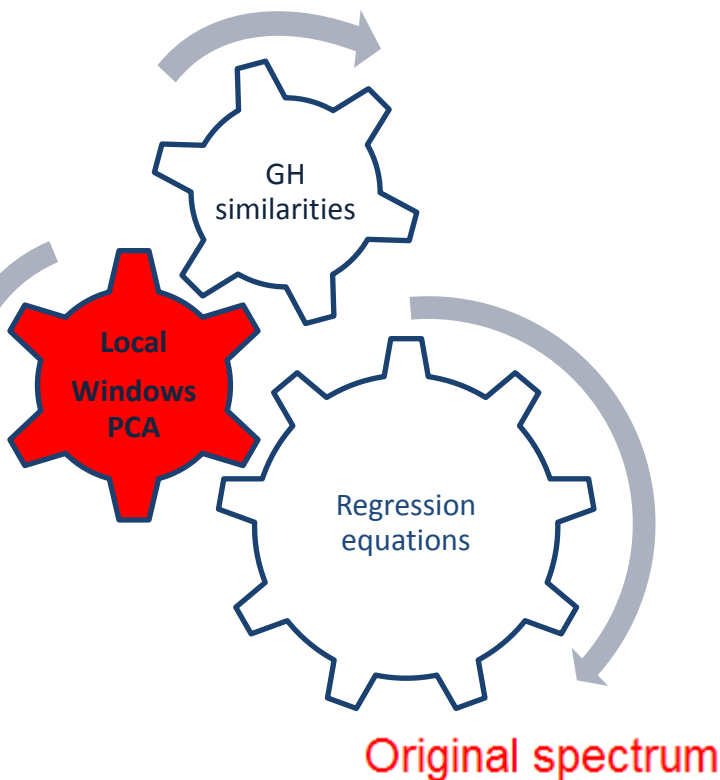
# Our "3 steps" strategy – regression equations

*Fernández Pierna, J.A., Abbas, O., Lecler, B., Hogrel, P., Dardenne, P., Baeten, V. (2015). NIR fingerprint screening for early control of non-conformity at feed mills. Food Chemistry, 189, pp. 2-12.*



# Our "3 steps" strategy – Local Windows PCA

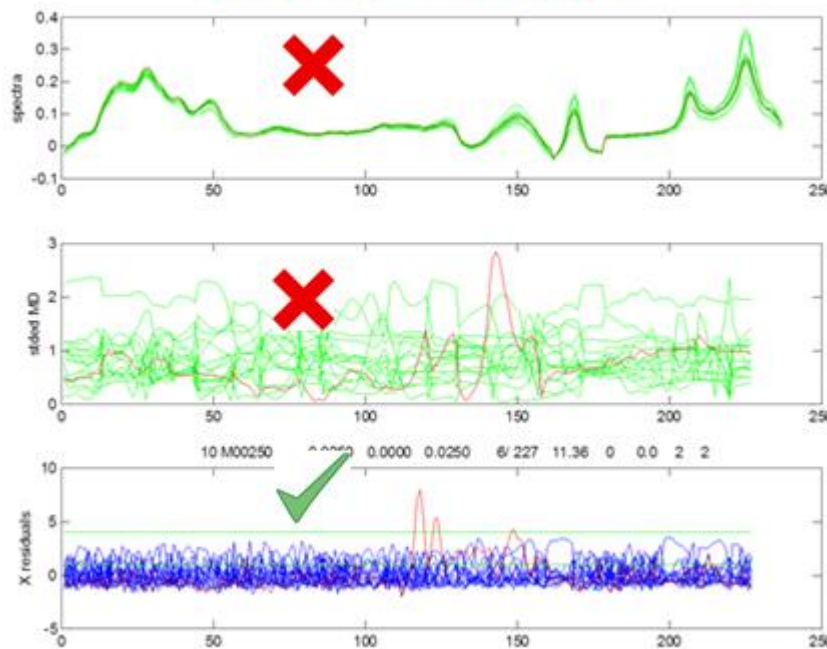
Fernandez Pierna, J.A. , Vincke, D. , Baeten, V. , Grelet, C. , Dehareng, F. & Dardenne, P. (2016). *Use of a multivariate moving window PCA for the untargeted detection of contaminants in agro-food products, as exemplified by the detection of melamine levels in milk using vibrational spectroscopy. Chemometrics and intelligent laboratory systems, 152, 157-162.*



GH (Mahalanobis dist.)

LWPCA

0.025% = 250ppm



# Tsunami of data – how to proceed?





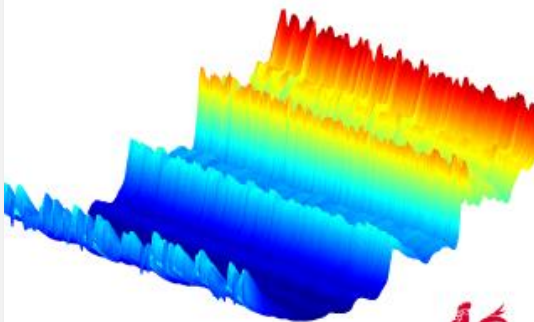
# Vibrational Spectroscopy and Chemometrics

Training Session

13 March–17 March 2017



Anniversary  
10<sup>th</sup>  
Edition



## The audience

The training is technical and practical and dedicated to participants with none or little knowledge in vibrational spectroscopy and chemometrics. Dedicated sessions could be organized for people with some knowledge on the methods.

## Chemometrics applied to vibrational data

Exploratory analysis

Data visualisation

Principal component analysis

Outlier detection

Uncertainty estimation

Quantification and classification

Multivariate calibration

Partial Least squares PLS

Multiple linear regression MLR

Support vector machines SVM

## List of speakers



**Ian Murray**

**Paolo Berzaghi**

**Tom Fearn**

Abbas, Ouissam (MIR spectroscopy)

Baeten, Vincent (Raman / Sampling)

Dardenne, Pierre (NIR considerations)

Fernández Pierna, Juan Antonio (Chemometrics)

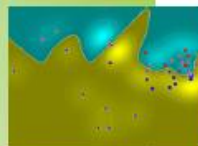
Vermeulen, Philippe (Hyperspectral Imaging)

Vincke, Damien (Hyperspectral Imaging)

Lecler, Bernard (Transfer/Standardization)

Minet, Olivier (NIR networks)

Sinnaeve, Georges (NIR online)



Anniversary  
10<sup>th</sup>  
Edition

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Centre wallon de Recherches agronomiques

25



Wallonie

# The Food and Feed Unit



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M. Caroline Lecrenier



Pierre Dardenne  
Head of Department



Zio Drissa



Quentin Ledoux



Olivier Minet



Philippe Vermeulen



Pascal Veys



Damien Vincke



Quentin Arnould



Stéphane Brichard



Claudine Clément



Marie Collard



Nicolas Crasset



Eric Fontaine



Nicalise Kayoka



Sandrine Mauro



Benoit Scout

+ Frédéric Dehareng et Clément Grelet (Unit 14, CRA-W)

# CLOUD SPECTROSCOPY

