



## Milk mid-infrared spectrometry: Take information from light

Soyeurt H.

# Gembloux Agro-Bio Tech, it is ...





- ▶ An **expertise** in fields related to the **life science** and the **bio-engineering**





- ▶ 1,378 students
  - 41 % of **students**
  - 32 % of **foreign students**
  - 40 **nationalities**
  - 327 **PhD students**

(statistics from May 2018)



- ▶ 499 members in the staff
  - 307 **researchers**
  - 44 **professors**
  - 61 **assistants**

(statistics from May 2018)



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# Milk MIR spectrometry

Context ...



Qu~~X~~ta



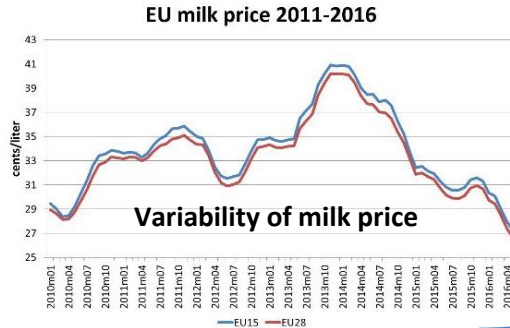




Increase of feeding cost

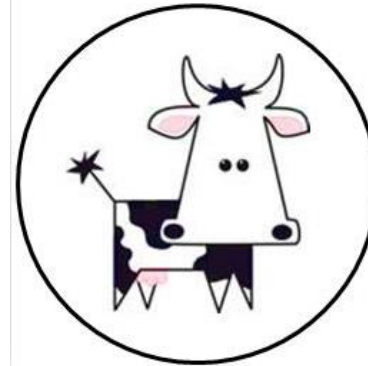


Environmental pressure



Milk composition is

- Part of economic outcome
- Mirror of the cow health



Optimize the production cost !!

Interest of developing decision tools from milk composition





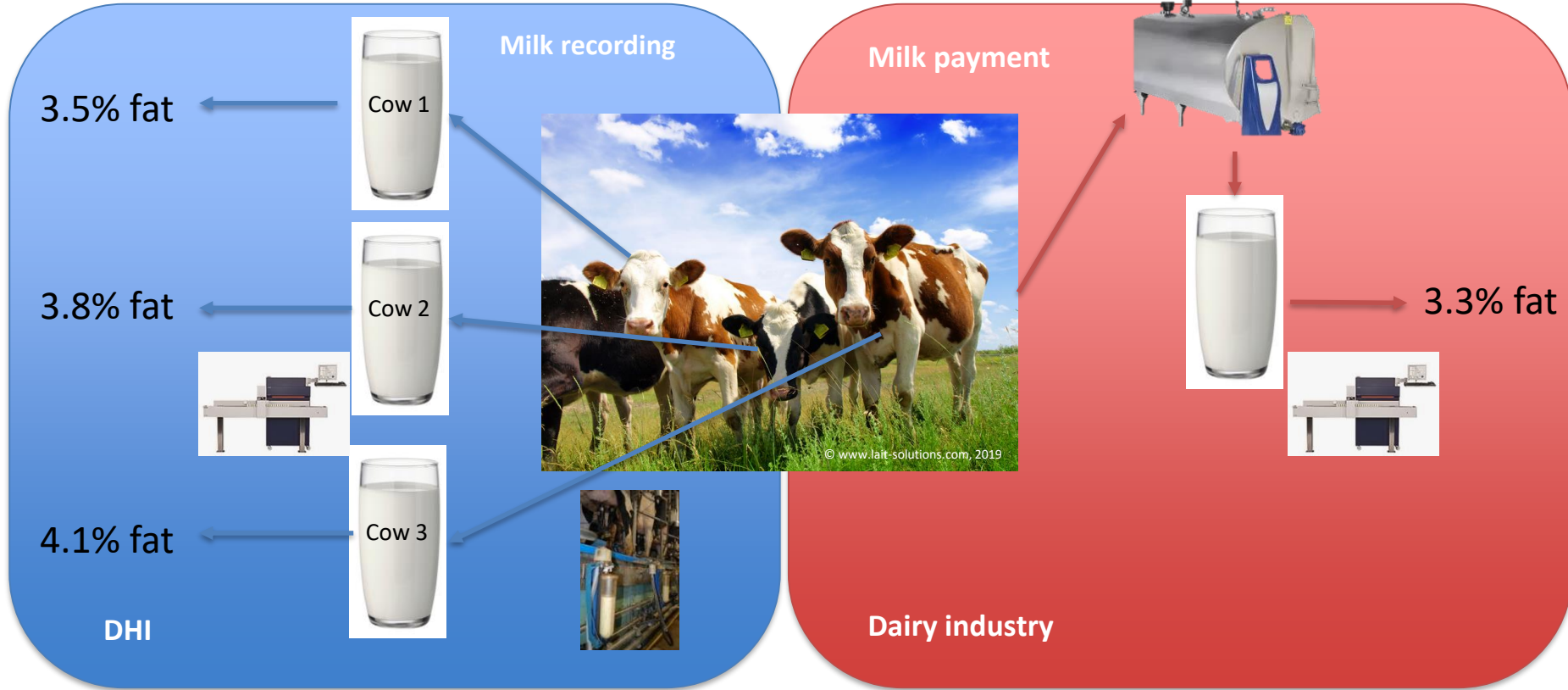
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# Milk MIR spectrometry

Milk analysis ...



# Milk sampling scheme



# Milk analysis

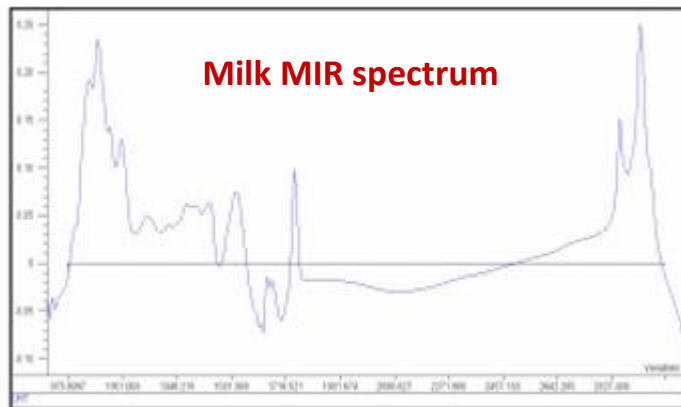


Milk recording  
(± 4 weeks for each cow)

Milk payment  
(± 3 days from bulk)



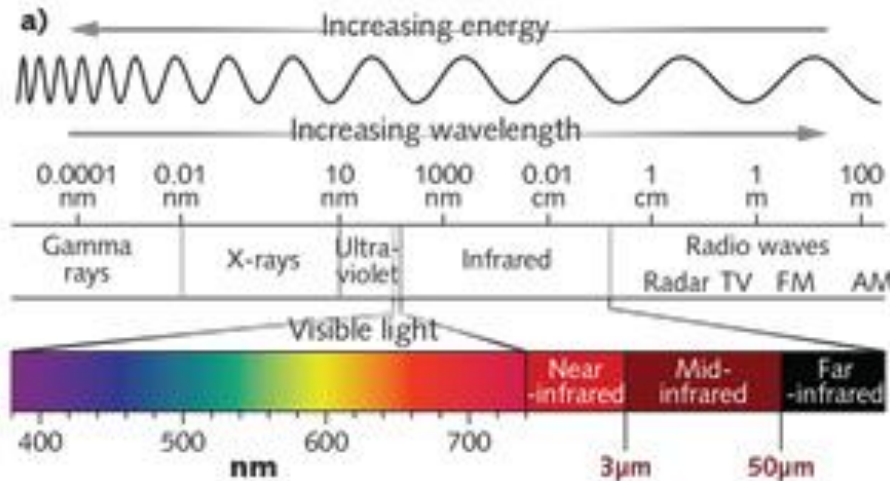
%fat





# What is Mid-Infrared (MIR) spectrum ?

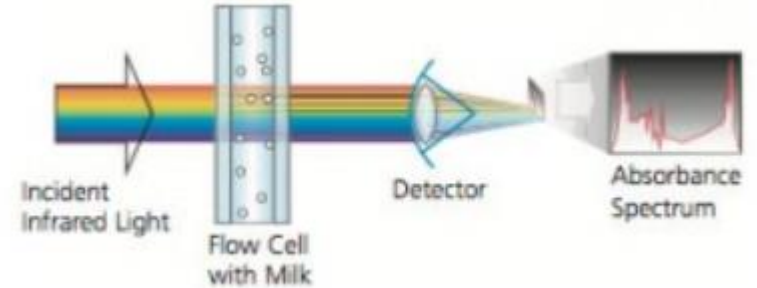
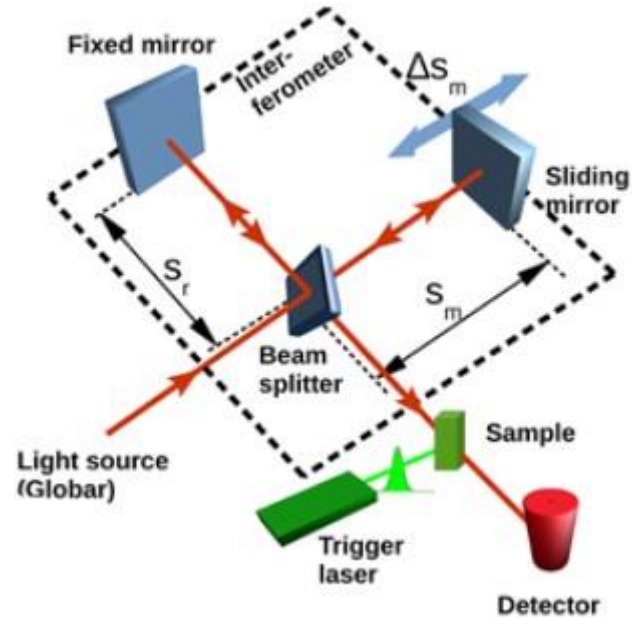
Electromagnetic radiation located between 3 and 50  $\mu\text{m}$



© Seddon et al., 2016, bioOptics world

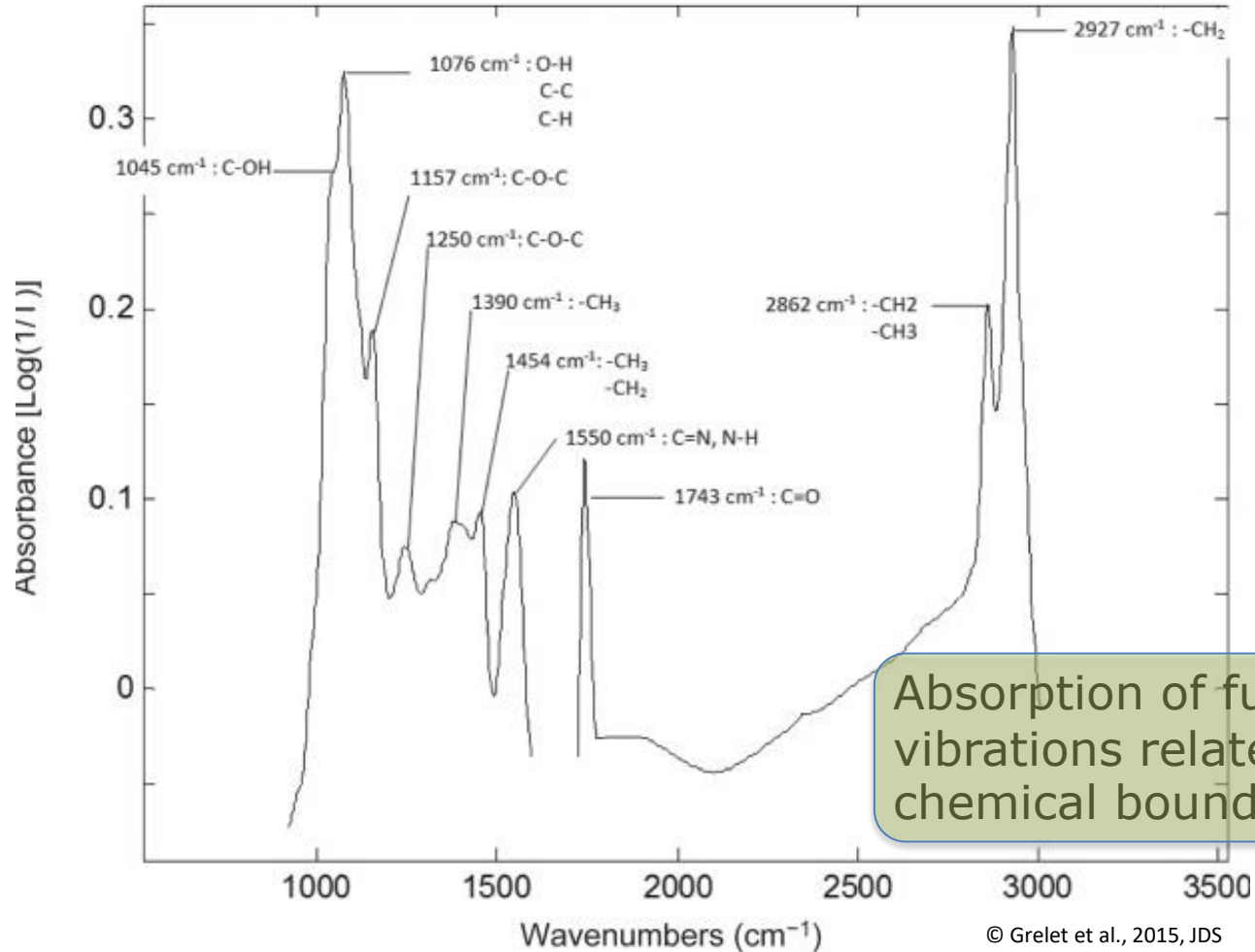


# What is MIR spectrometry?

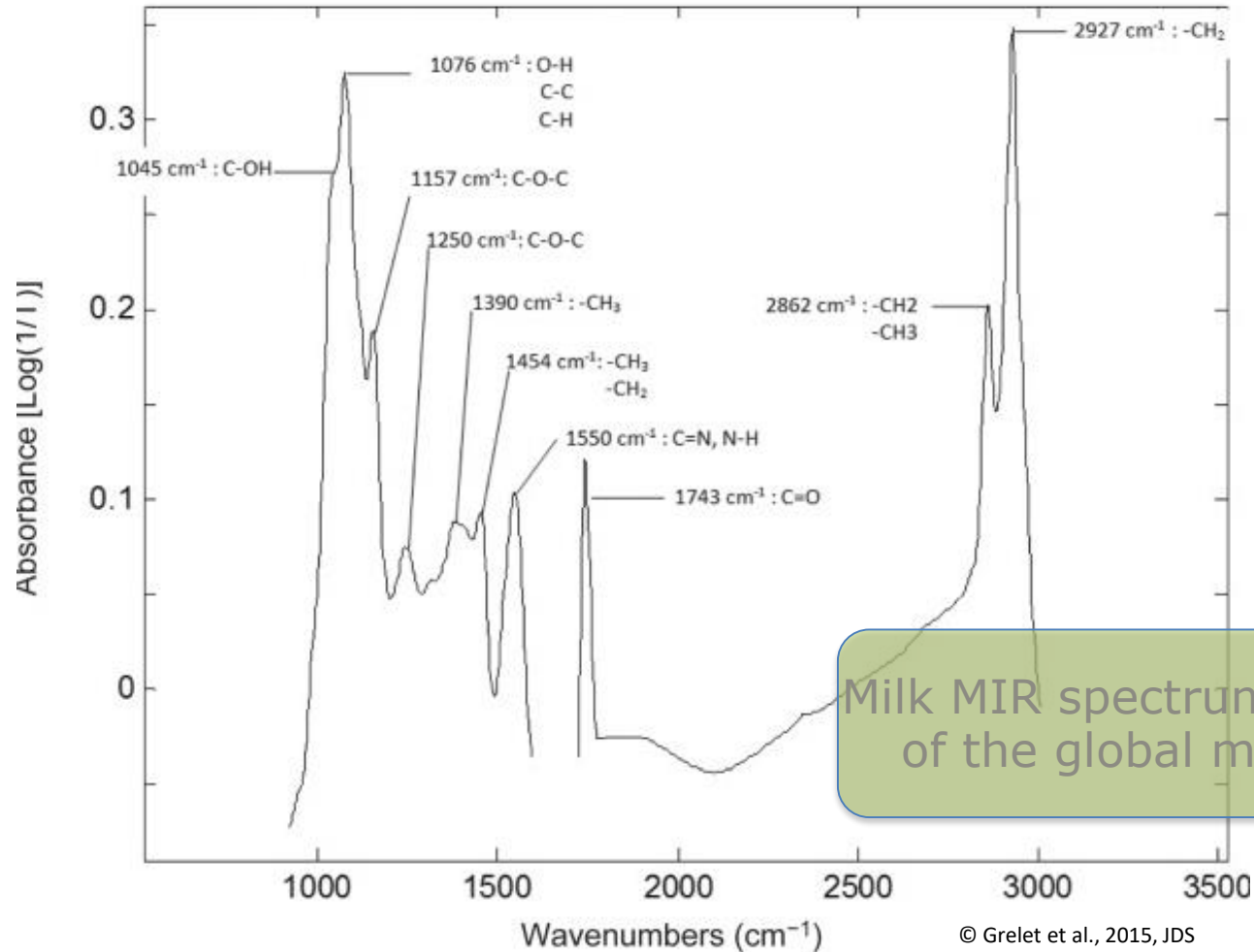


© Bentley instrument, 2019

© Ritter et al., 2015, Frontiers in Molecular Biosciences



Absorption of fundamental vibrations related to specific chemical bounds within a molecule



Milk MIR spectrum is representative of the global milk composition.





# Different brands

## Perten (Delta)



© Foss website, 2019

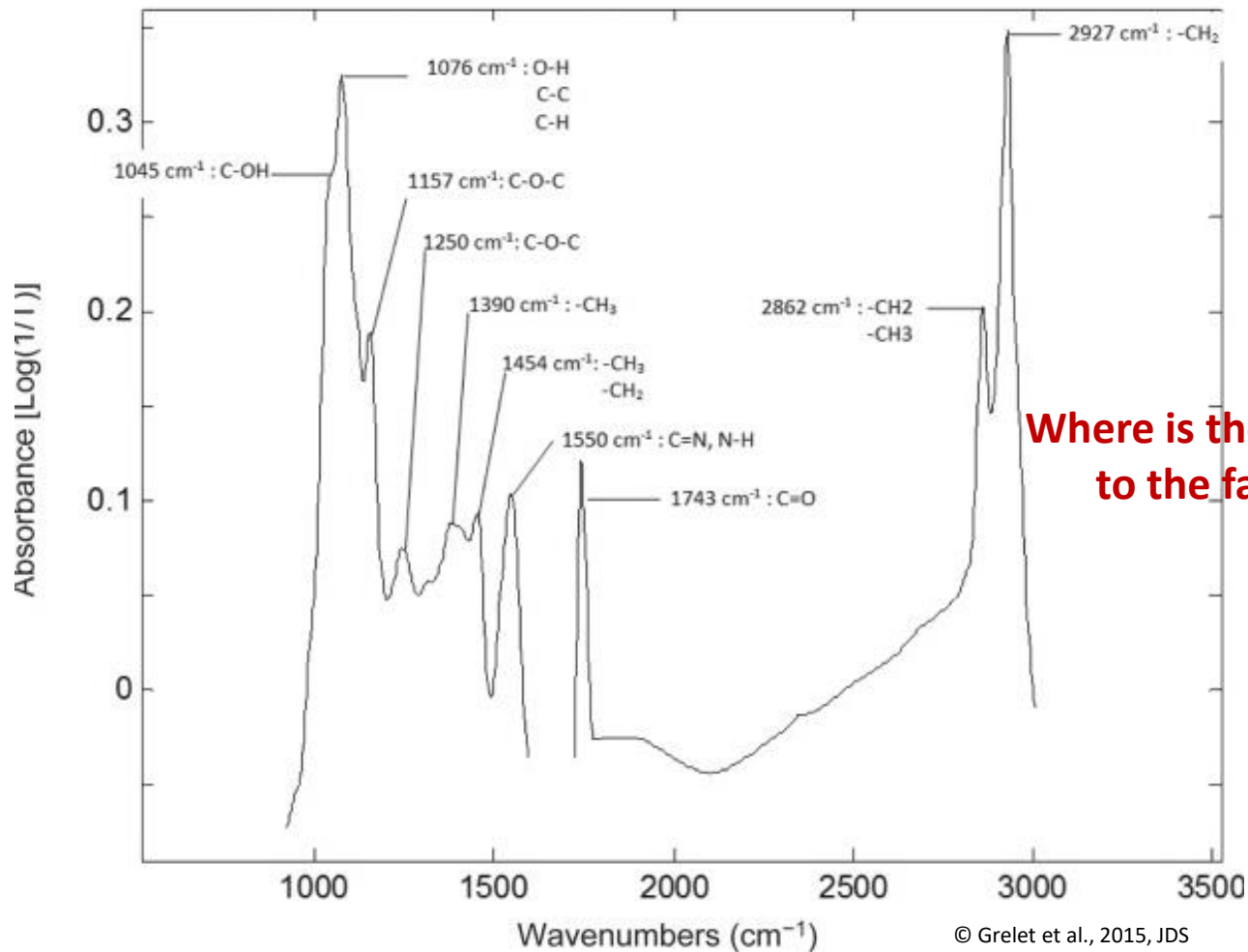


© Bentley instrument website, 2019



© Perten instrument website, 2019

- Different **resolutions**
- Different **spectral ranges**



**Where is the information related to the fat quantification ?**



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## Milk MIR spectrometry

How to extract the interesting information ...

# Milk analysis



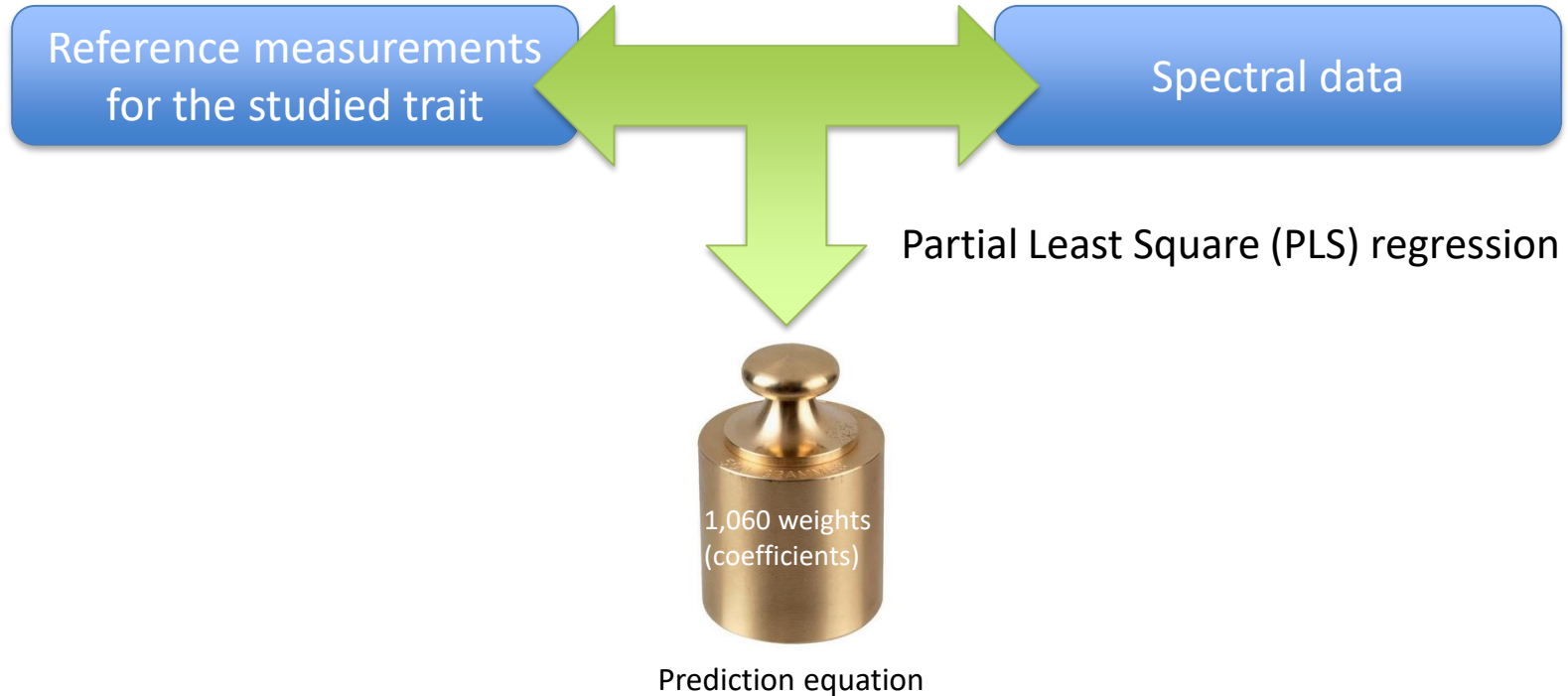
Prediction equation

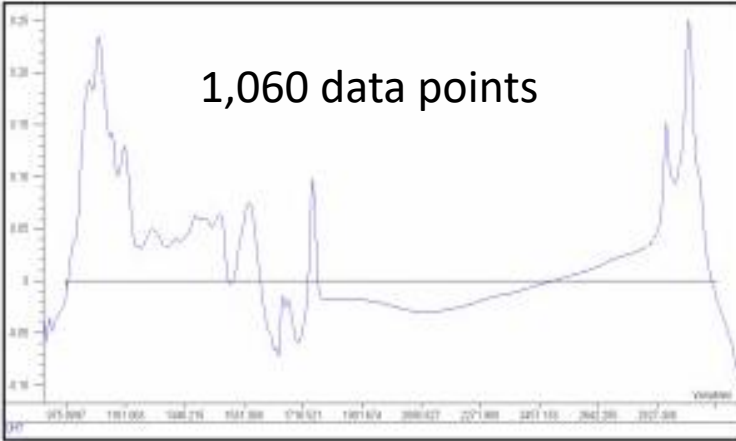
Milk recording  
(± 4 weeks for each cow)

Milk payment  
(± 3 days from bulk)



# How to build a prediction equation





1,060 data points

Spectra with unknown reference measurements

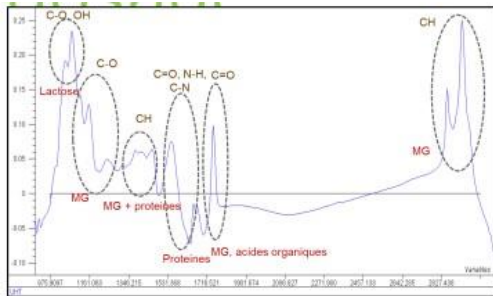


1,060 weights  
(coefficients)

Prediction equation

More than 17 millions of test day records

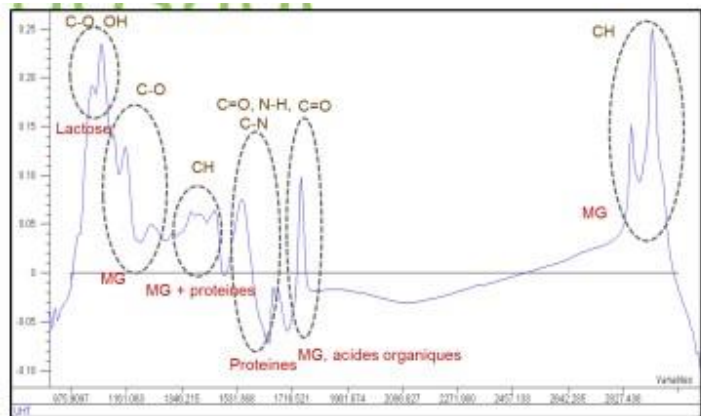
Prediction for new spectra



Prediction equation



- Before 2005, only equations related to **fat** and **proteins** were implemented in all milk laboratories
- In some others, equations were available also for **lactose** and **urea**
- **Walloon research team** composed by Gembloux Agro-Bio Tech, Walloon Research Centre, Comité du Lait and Walloon Breeding Association (Awé) through FuturoSpectre decided to **extend the use of milk MIR spectral data**
- In 2005, they were the **first to record the spectral data for DHI application**



Prediction equation



**Mid-infrared prediction of bovine milk fatty acids across multiple breeds, production systems, and countries**

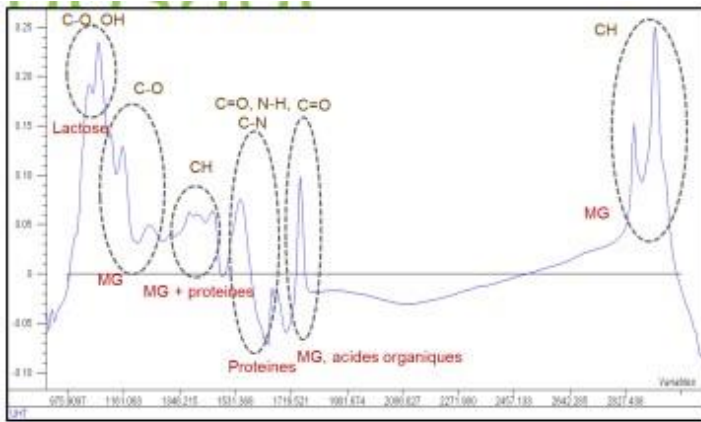
H. Soyeurt<sup>1,1</sup>, F. Dehareng<sup>2</sup>, N. Gengler<sup>1</sup>, S. McParland<sup>3</sup>, E. Wall<sup>2</sup>, D.P. Berry<sup>5</sup>, M. Coffey<sup>6</sup>, P. Dardenne<sup>2</sup>  
 Show more

<http://dx.doi.org/10.3168/jds.2010-3408>

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Prediction equation





**Journal of Dairy Science**

Volume 92, Issue 6, June 2009, Pages 2444–2454



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Research-article

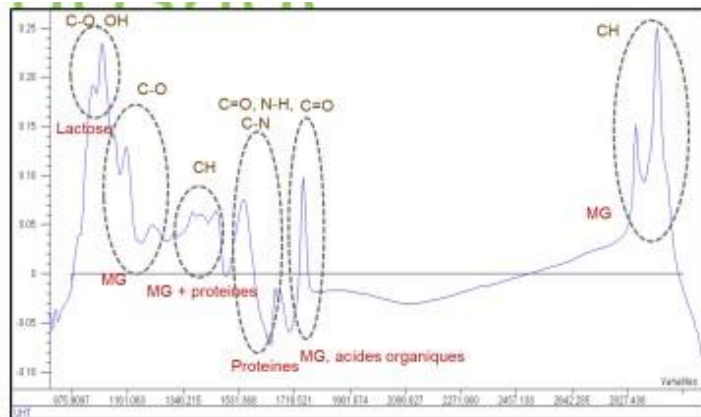
### Potential estimation of major mineral contents in cow milk using mid-infrared spectrometry

H. Soyeurt<sup>1</sup>, D. Bruwier<sup>2</sup>, J.-M. Romnee<sup>3</sup>, N. Gengler<sup>1,4</sup>, C. Bertozzi<sup>5</sup>, D. Veselko<sup>6</sup>, P. Dardenne<sup>7</sup>

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<http://dx.doi.org/10.3168/jds.2008-1734> [Get rights and content](#)





Prediction equation



animal, Volume 6, Issue 11

November 2012, pp. 1830-1838

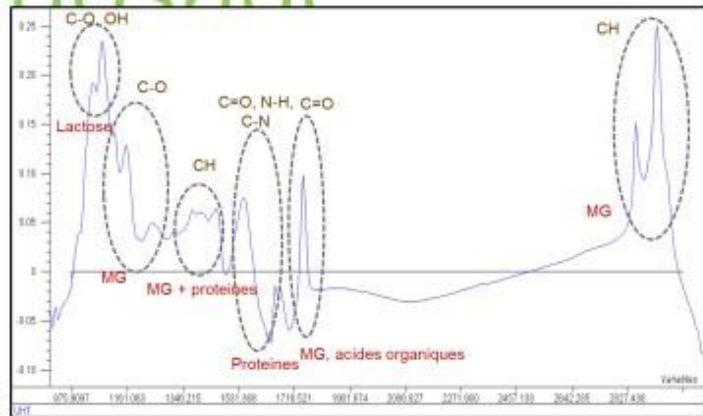
## Mid-infrared prediction of lactoferrin content in bovine milk: potential indicator of mastitis

H. Soyeurt <sup>(a1)</sup> <sup>(a2)</sup>, C. Bastin <sup>(a1)</sup>, F. G. Colinet <sup>(a1)</sup>, V. M.-R. Arnould <sup>(a1)</sup> <sup>(a3)</sup>, D. P. Berry <sup>(a4)</sup>, E. Wall <sup>(a5)</sup>, F. Dehareng <sup>(a6)</sup>, H. N. Nguyen <sup>(a6)</sup>, P. Dardenne <sup>(a6)</sup>, J. Schefers <sup>(a7)</sup>, J. Vandenplas <sup>(a1)</sup> <sup>(a2)</sup>, K. Weigel <sup>(a7)</sup>, M. Coffey <sup>(a5)</sup>, L. Théron <sup>(a8)</sup>, J. Detilleux <sup>(a8)</sup>, E. Reding <sup>(a9)</sup>, N. Gengler <sup>(a1)</sup> <sup>(a2)</sup> and S. McParland <sup>(a4)</sup> 

DOI: <http://dx.doi.org/10.1017/S1751731112000791>

Published online: 01 April 2012



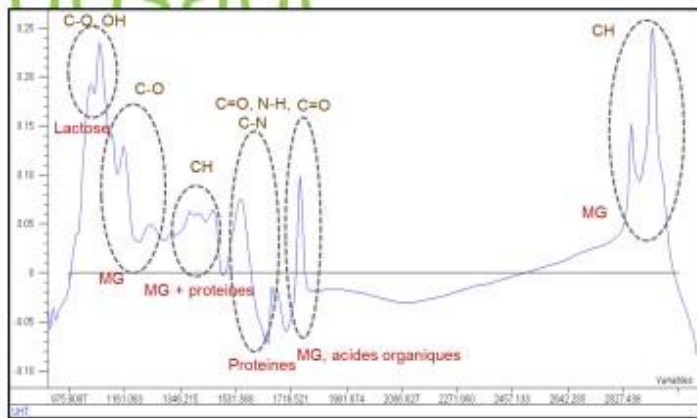


Prediction equation



If you **increase** the number of **prediction equations**, you can **increase** the number of **phenotypes** based on the **same** raw **spectra**

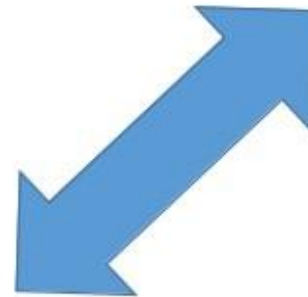
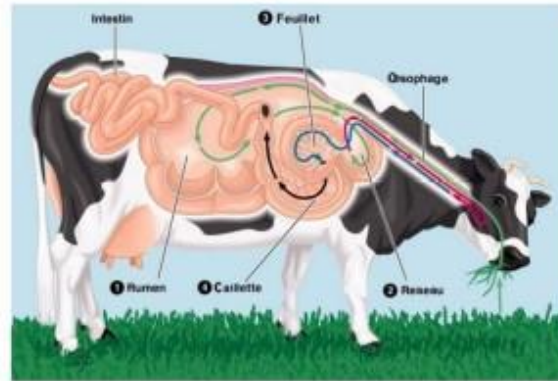
# More than just a prediction related to milk composition



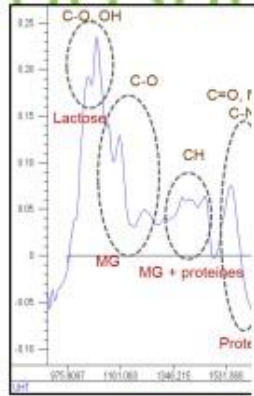
Prediction equation



Indirect links with **cow** metabolic **status**



# More than just a prediction related to milk composition



Development of Fourier transform mid-infrared calibrations to predict acetone,  $\beta$ -hydroxybutyrate, and citrate contents in bovine milk through a European dairy network

C. Grelet<sup>1</sup>, C. Bastin<sup>1</sup>, M. Gelé<sup>1</sup>, J.-B. Davière<sup>1</sup>, M. Johan<sup>1</sup>, A. Werner<sup>2</sup>, R. Reding<sup>1</sup>, J.A. Fernandez Pierna<sup>3</sup>, F.G. Colinet<sup>4</sup>, P. Dardenne<sup>5</sup>, N. Gengler<sup>6</sup>, H. Soyeurt<sup>7</sup>, F. Dehareng<sup>8</sup>

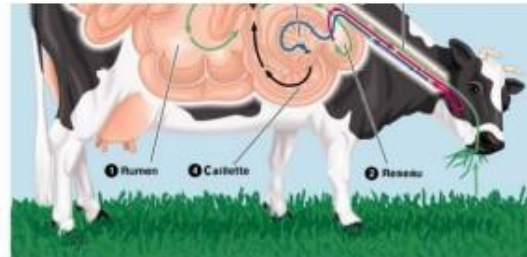
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<http://dx.doi.org/10.3168/jds.2015-10477>

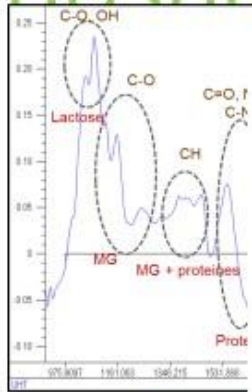
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Energy balance  
Acidosis



# More than just a prediction related to milk composition




Journal of Dairy Science

Volume 98, Issue 8, August 2015, Pages 5740–5747



**Hot topic: Innovative lactation-stage-dependent prediction of methane emissions from milk mid-infrared spectra**

A. Vanlierde<sup>a, 1</sup>, M.-L. Vanrobays<sup>a, 1</sup>, F. Dehareng<sup>a</sup>, E. Froidmont<sup>a</sup>, H. Soyeurt<sup>a</sup>, S. McParland<sup>b</sup>, E. Lewis<sup>b</sup>, M.H. Deighton<sup>a</sup>, F. Grand<sup>a</sup>, M. Kreuzer<sup>a</sup>, B. Gredler<sup>a</sup>, P. Dardenne<sup>a</sup>, N. Gengler<sup>a</sup>  

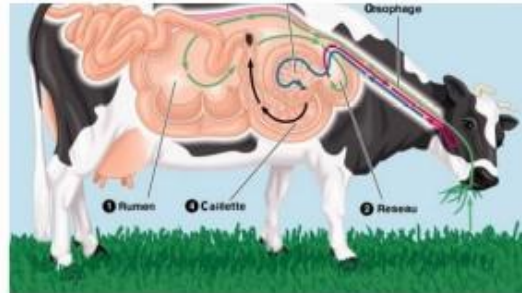
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<http://dx.doi.org/10.3168/jds.2014-8436>

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Energy balance  
Acidosis  
Methane ...





## Increasing the use of MIR

- ▶ Other developments
  - Cheese making properties
  - Detection of abnormal milk
  - ...
- ▶ Obtaining MIR spectral data is **computationally easy**
- ▶ Allowing the developments of **management and breeding** tools thanks to its **high throughput**



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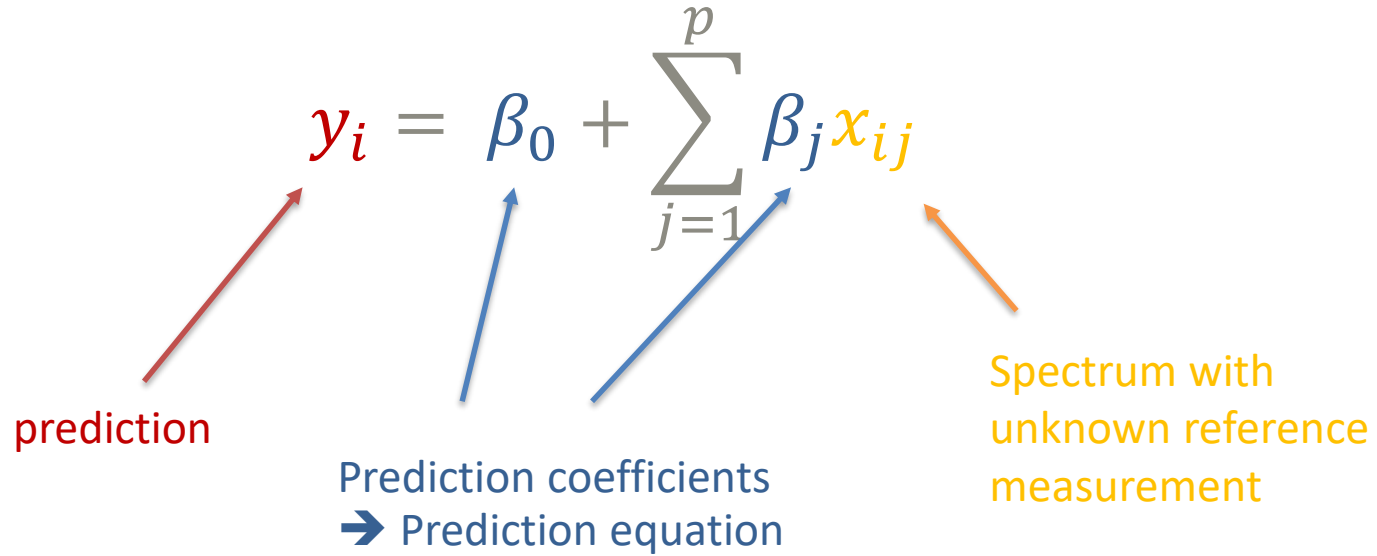
## Milk MIR spectrometry

Need to have high quality predictions ...



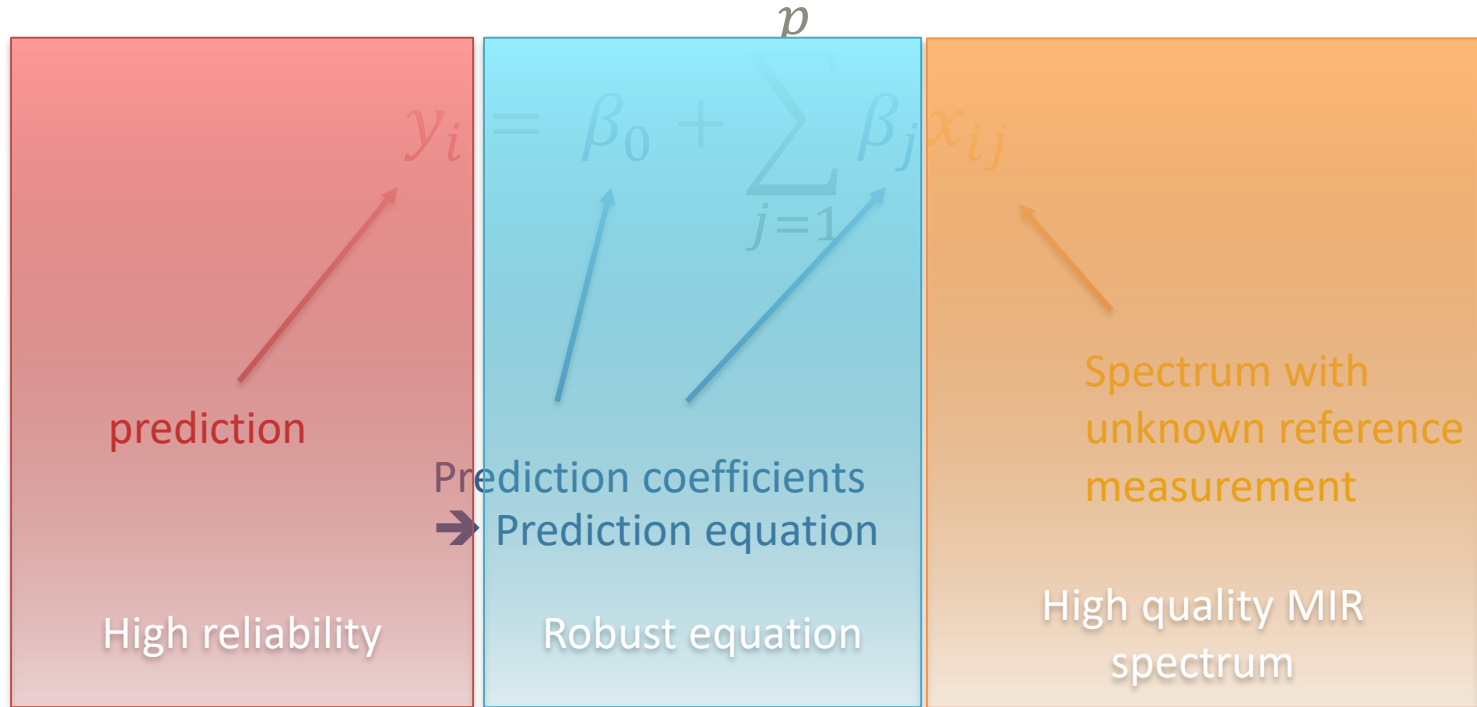


# Obtaining of reliable predictions



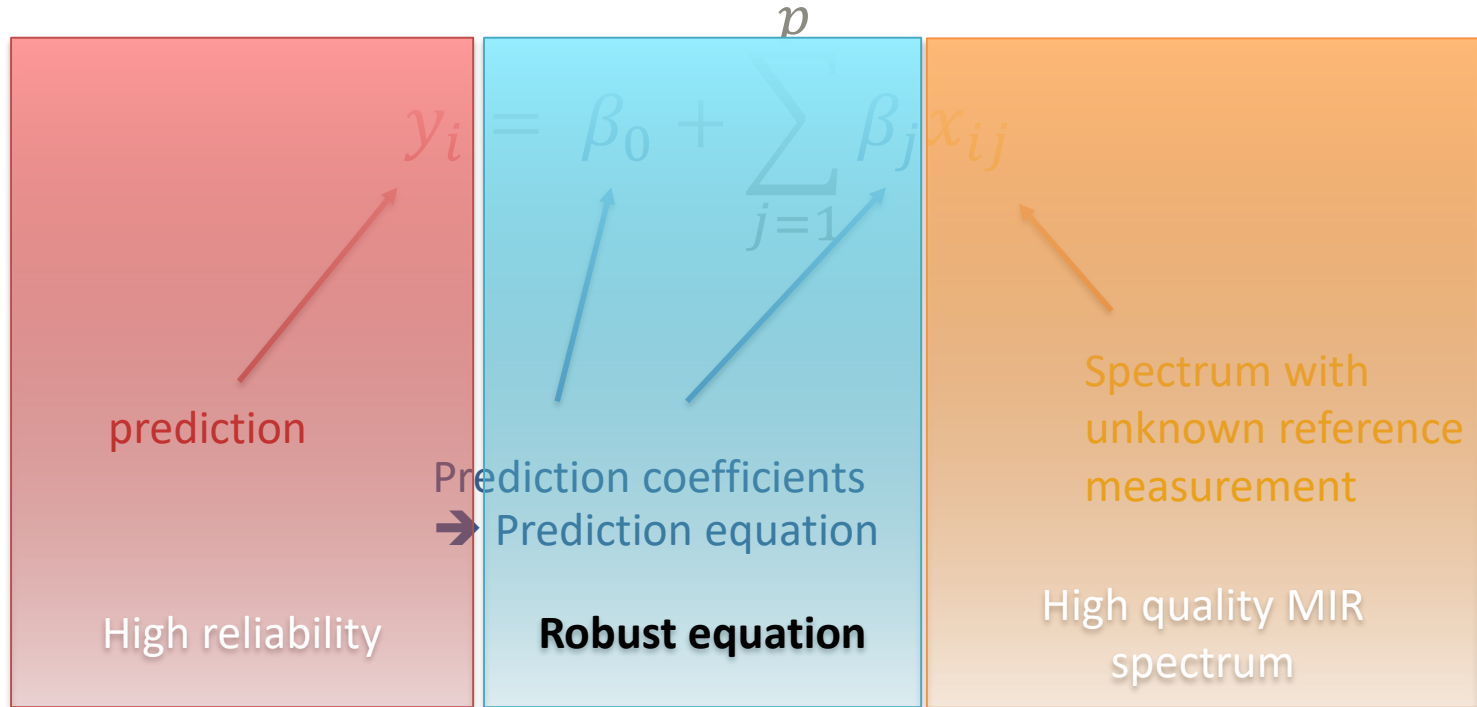


# Obtaining of reliable predictions





# Obtaining of reliable predictions





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## Milk MIR spectrometry

Need to have robust prediction equations ...



# How to build a robust prediction equation

- ▶ Structure of the **calibration set** to estimate the coefficients
  - reference data used to estimate the coefficients of the established prediction equations
- ▶ **Accuracy** of the prediction
  - estimated from one or several sets of independent samples.



## Structure of calibration set

- ▶ **Representative** of the dairy cattle population where the prediction equation will be applied
- ▶ Covering the **maximum variability** to avoid extrapolation
  - If a part of the variability of the spectral data and/or the studied trait is missing, this leads to extrapolate the prediction
  - Increasing the chance to decrease the expected accuracy



## Accuracy of the prediction

- ▶ **Independent** validation set
  - Not always satisfy due to practical or financial issues
  - Repeated measurements per animal, herd, season ...
- ▶ The cross-validation can overestimate the prediction accuracy if the independency is not verified
- ▶ So, it is always required to **know the methodology used to estimate the accuracy** of a prediction given by an equation.



# How to build a robust prediction equation

- ▶ Structure of the **calibration set** to estimate the coefficients

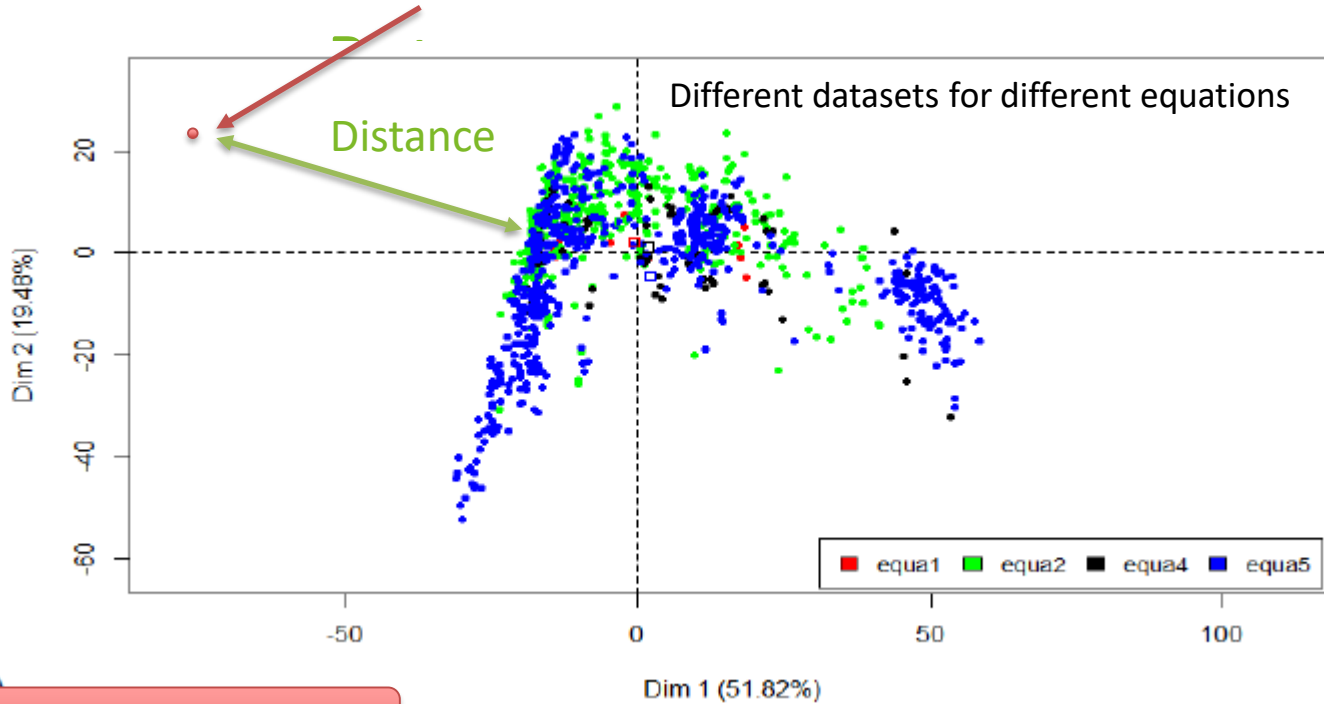
The elements available for the milk laboratories are often too limited to assess the robustness of a prediction equation

- ▶ **Accuracy** of the prediction
  - estimated from one or several sets of independent samples.

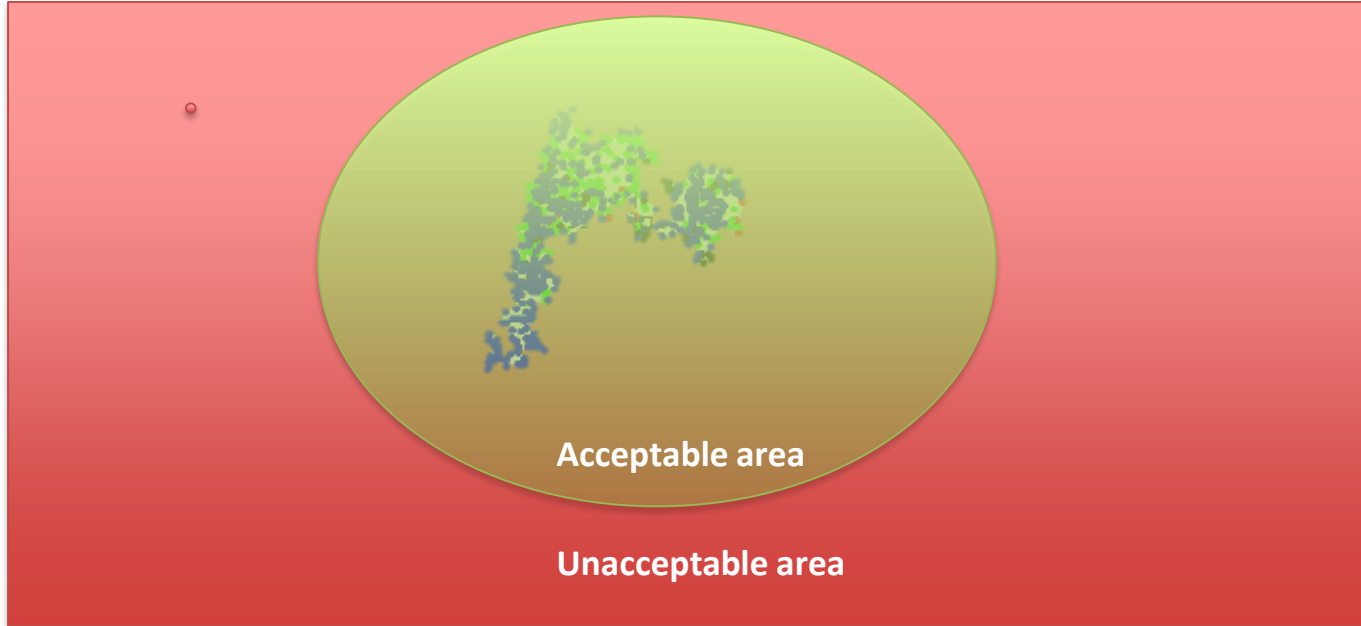




Can I make a prediction from this spectrum ?



No, because too far





## Limitation

- ▶ Need to limit the spectral extrapolation
- ▶ Need to assess the structure of the calibration set
  - Standardized Mahalanobis distance
    - › Distance lower than 3 reduced the risk of making a spectral extrapolation
  - Distance correlation
  - ...

This work is not done currently → Some extrapolation can be made without knowing that → biased prediction

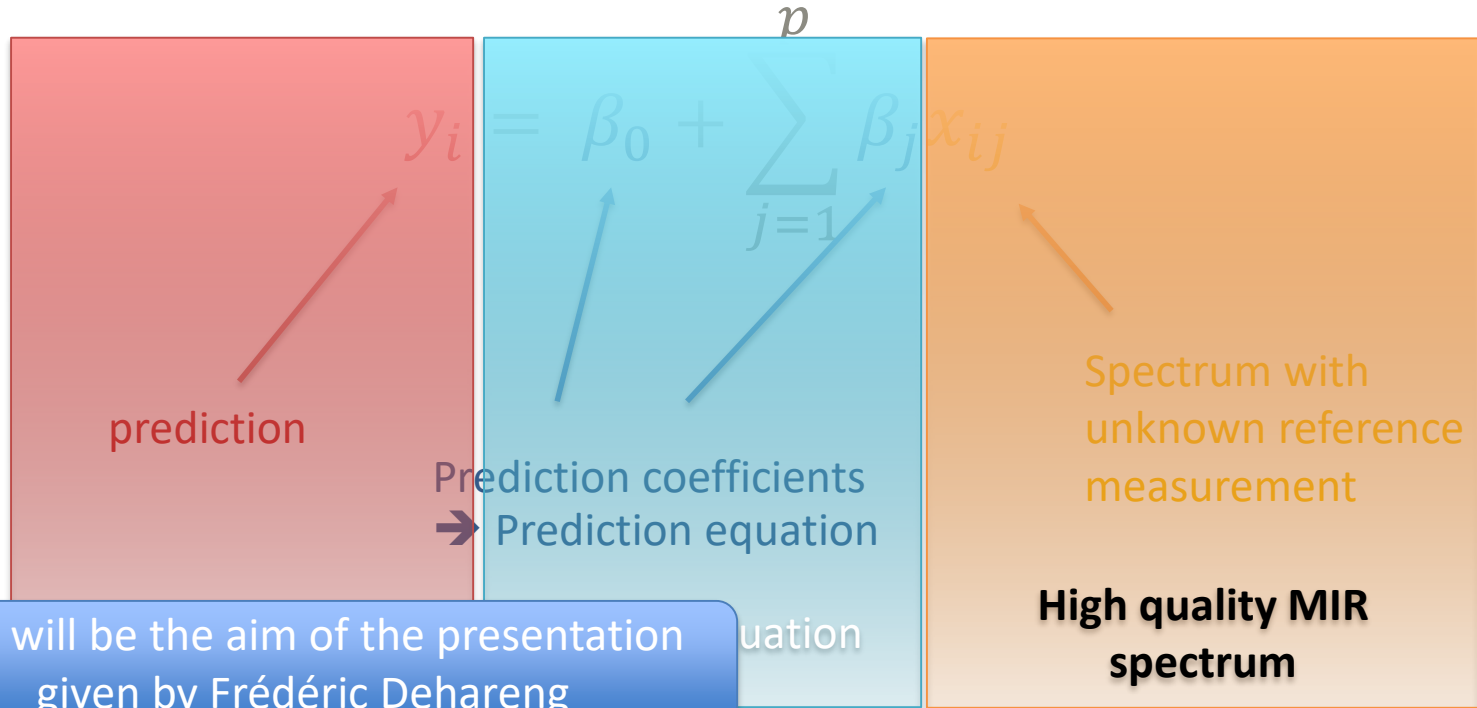


## Limitations

- ▶ Covering as much as possible the variability of the studied trait is **expensive**
  - Interest to create international network to develop equations
    - › Decreasing the research costs
    - › Sharing knowledge
    - › Limiting the existence of different equations for the same trait with variable accuracy



# Obtaining of reliable predictions



This will be the aim of the presentation given by Frédéric Dehareng



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# Milk MIR spectrometry

Conclusions ...



## Conclusions

- ▶ **High interest** for using milk MIR spectrometry to develop management and breeding tools
- ▶ Technology **already implemented** in all milk laboratories
- ▶ Establish a **guide of good practises** to ensure a high quality of predictions
  - International Committee for Animal Recording (ICAR)
  - International dairy federation (IDF)
- ▶ **Promoting international collaborations** for the development of prediction equations



## Milk mid-infrared spectrometry: Take information from light

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Thank you for your attention