How mid-infrared spectroscopy of milk could contribute to improve the sustainability of the dairy sector

Frédéric Dehareng[1], Clément Grelet[1] & Amélie Vanlierde[2]

[1]Quality and authentication of agricultural products Unit, CRA-W
[2]Animal production Unit, CRA-W

IDF BENC Event, Connection and Interaction between Research and Practice, 18th April 2024

If we want to understand and effectively manage sustainability, it requires having a large amount of standardized data/measurements, that accurately represent its complexity, diversity and evolution

… and if possible not too expensive

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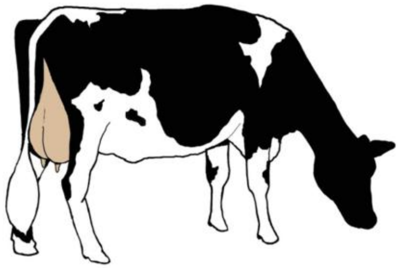
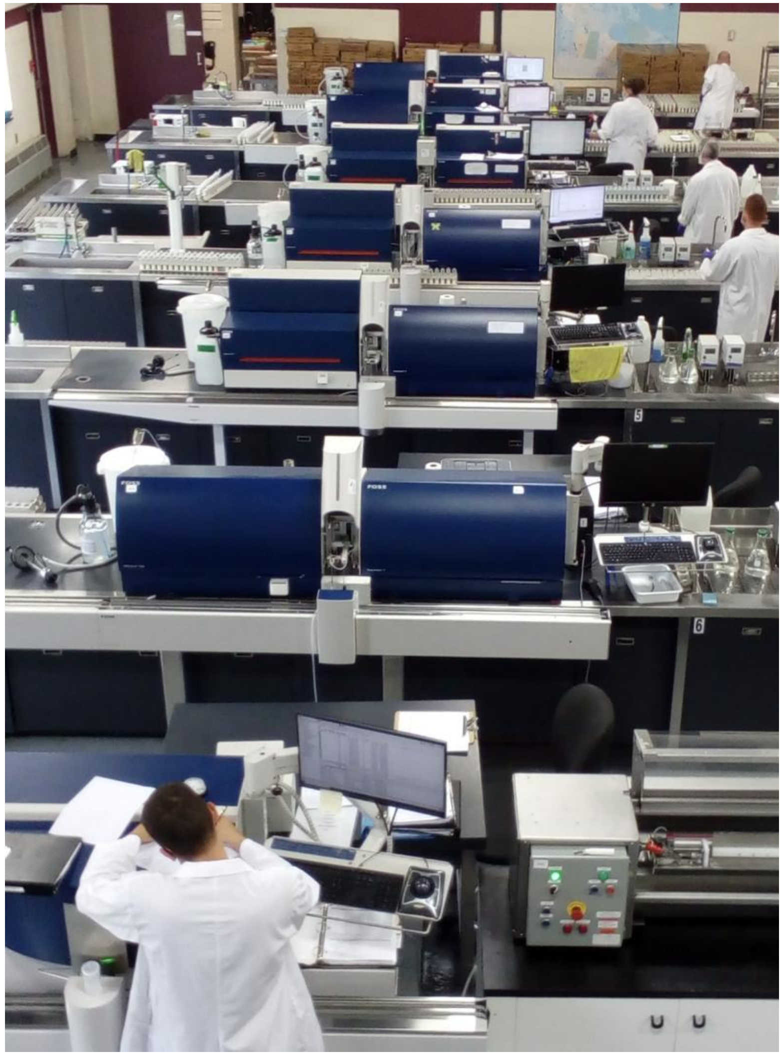
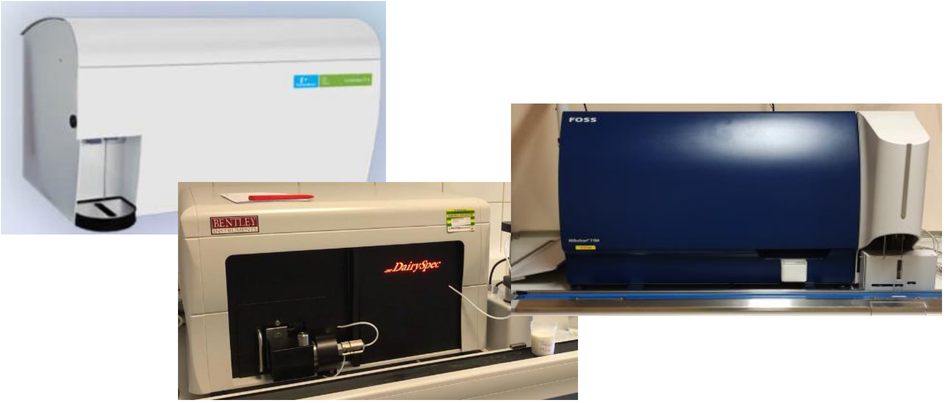


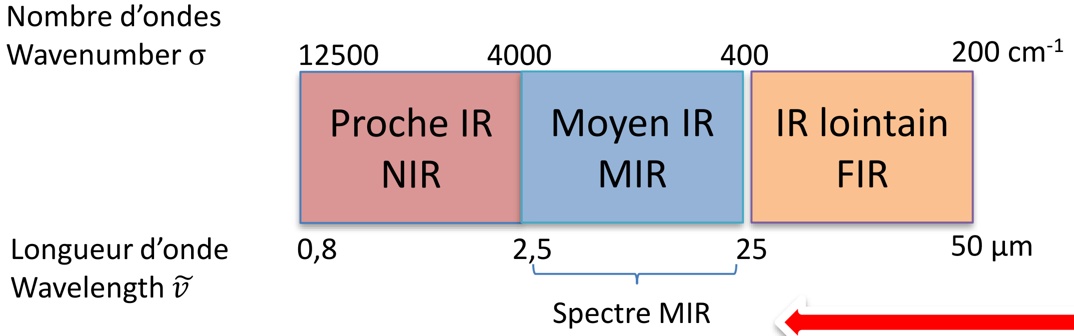
… and if possible not too expensive

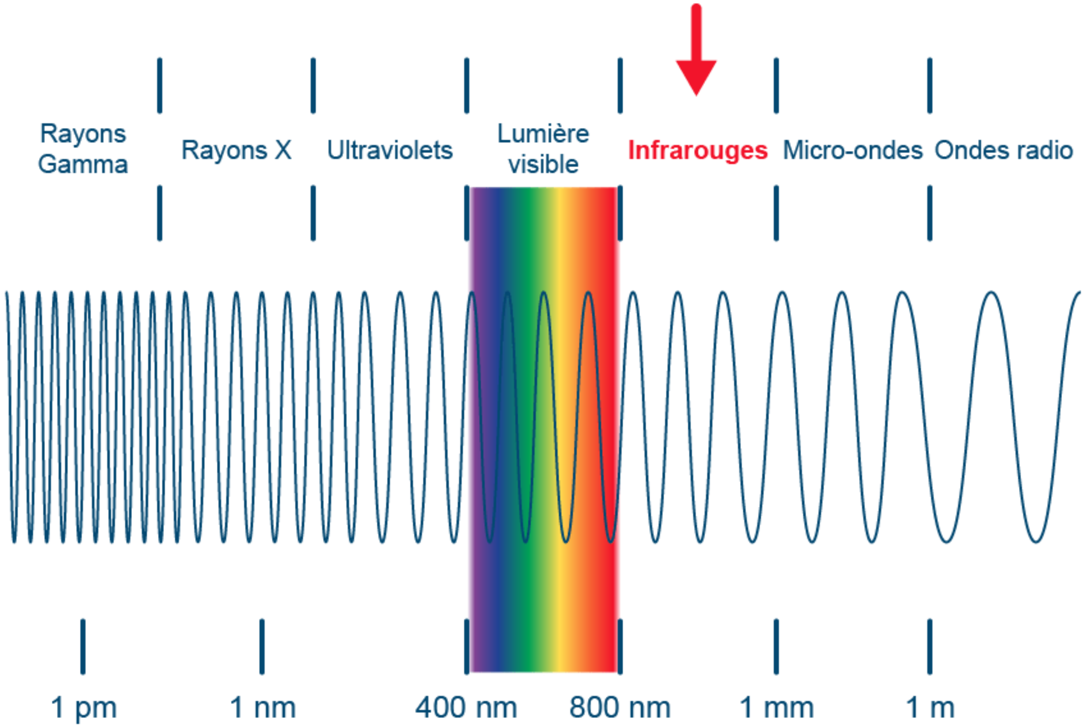


- Milk recording
- Milk payment
- During the process

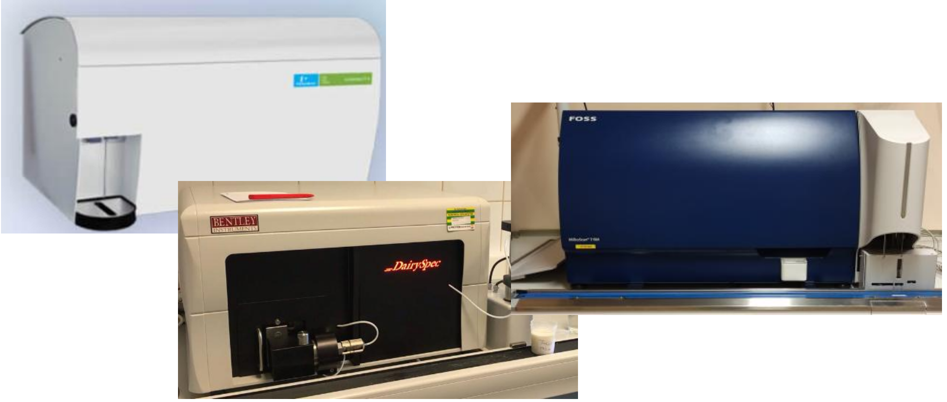
What is mid-infrared Spectroscopy ?







What is mid-infrared Spectroscopy ?



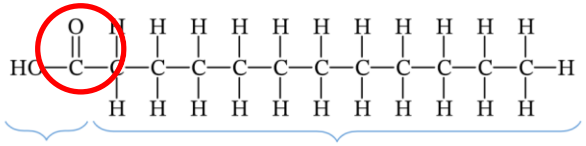
Nombre d'ondes
Wavenumber σ

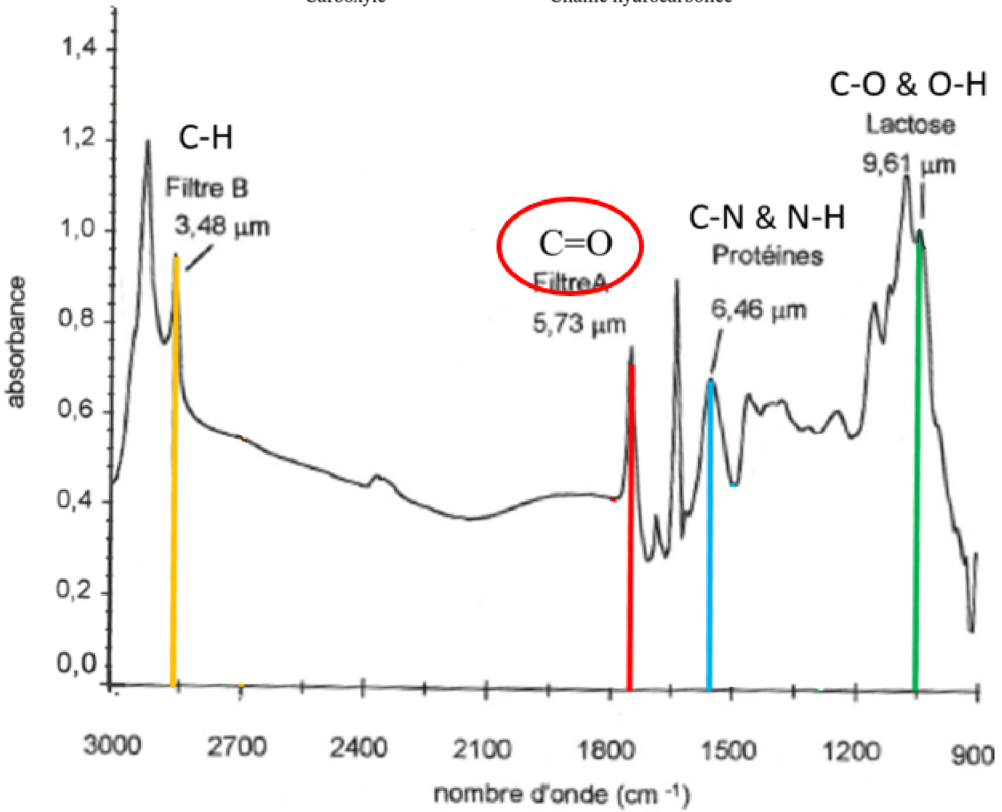
$\sigma = 1/\tilde{\upsilon}$

12500	4000	400	200 cm^{-1}
Proche IR NIR	Moyen IR MIR	IR lointain FIR	
0,8	2,5	25	50 µm

Longueur d'onde
Wavelength $\tilde{\upsilon}$

Spectre MIR





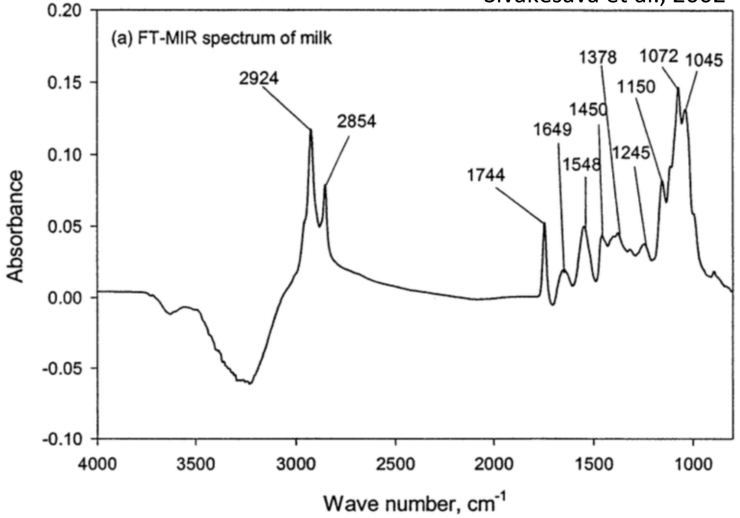
(d'après Bertrand et Dufour, 2000)

$$\begin{cases} a_{1,1}x_1 + a_{1,2}x_2 + \ldots + a_{1,n}x_n = b_1 \\ a_{2,1}x_1 + a_{2,2}x_2 + \ldots + a_{2,n}x_n = b_2 \\ \vdots \\ \vdots \\ a_{m,1}x_1 + a_{m,2}x_2 + \ldots + a_{m,n}x_n = b_m \end{cases}$$

FT-MIR models

- Direct models
- Indirect models
- Pseudo-direct models
- Others

Sivakesava et al., 2002



To estimate models quality -> Clustering based on RPD, RMSE and R^2

Model quality	RPDcv	Relative RMSEcv	R^2cv	Interpretation for application
1	+ 6	<5%	>0.97	Any application
2	4.2 - 6	<10%	>0.94	Quality control
3	3 - 4.2	<10%	>0.89	Quantitative screening
4	2 - 3	<25%	>0.74	Rought screening
5	1.5 - 2	<25%	>0.55	Allows to compare groups, discriminate high or low values
6	1.5 - 2	>25%	>0.55	Highly imprecise, can be used to detect extreme values
7	0 - 1.5	-	<0.55	Not recommended

Direct models e.g: FAT, PROT, LACTOSE… > 100 ppm ou mg/kg

Model quality
1

Major FATTY ACIDS

J. Dairy Sci. 94:1657–1667
doi:10.3168/jds.2010-3408

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

H. Soyeurt,*†[1,2] F. Dehareng,‡[1] N. Gengler,*† S. McParland,§ E. Wall,‡ D. P. Berry,§ M. Coffey,# and P. Dardenne‡
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§Teagasc Moorepark Dairy Production Research Centre, Fermoy, Co. Cork, Ireland
#Sustainable Livestock Systems Group, Scottish Agricultural College, Bush Estate, Penicuik, Midlothian, EH26 0PH, United Kingdom

- Nutritional quality
- Physical properties
- Cow status biomarkers (energy balance, rumination…)

Direct models

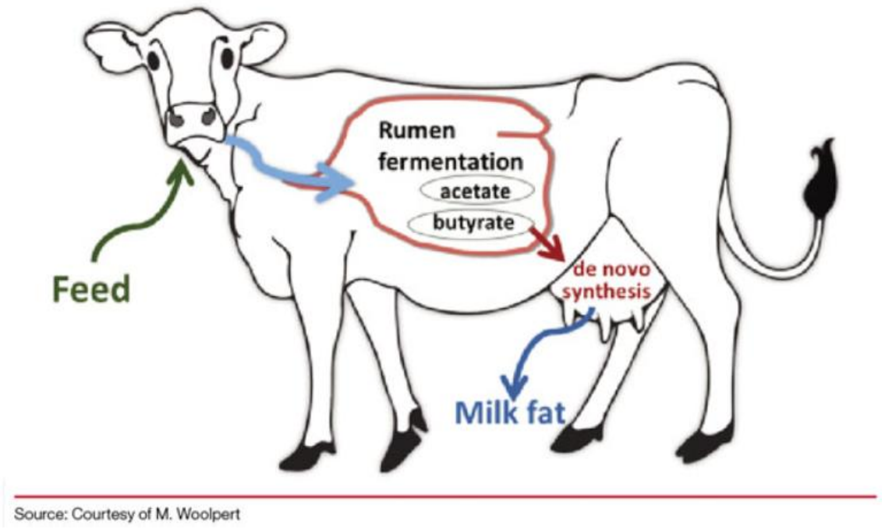
Groups of models		Predicted variable	Min	Max	Mean	SD	R²cv	Relative RMSEcv	RPDcv	Model quality
Milk Fatty acids	CRA-W, Ulg, Teagasc, SRUC, FCEL, LKV-BW, LKV-NRW, LUKE, Valio, LKV-Austria	Milk C4 (g/dL)	0.01	0.23	0.10	0.03	0.93	8%	3.67	3
		Milk C6 (g/dL)	0.01	0.16	0.07	0.02	0.91	9%	3.32	3
		Milk C8 (g/dL)	0.01	0.11	0.05	0.01	0.91	9%	3.29	3
		Milk C10 (g/dL)	0.02	0.32	0.11	0.04	0.91	9%	3.37	3
		Milk C12 (g/dL)	0.02	0.41	0.13	0.04	0.92	9%	3.62	3
		Milk C14 (g/dL)	0.05	1.20	0.45	0.13	0.93	7%	3.88	3
		Milk C14_1 (g/dL)	0.00	0.15	0.04	0.02	0.68	21%	1.78	5
		Milk C16 (g/dL)	0.12	3.32	1.20	0.40	0.94	8%	4.18	3
		Milk C16_1c (g/dL)	0.01	0.24	0.07	0.03	0.73	20%	1.91	5
		Milk C17 (g/dL)	0.00	0.09	0.03	0.01	0.80	13%	2.24	4
		Milk C18 (g/dL)	0.05	1.32	0.40	0.15	0.84	14%	2.51	4
		Milk C18_1cis9 (g/dL)	0.08	2.69	0.76	0.29	0.95	8%	4.35	2
		Milk C18_2c9c12 (g/dL)	0.00	0.17	0.06	0.02	0.72	19%	1.91	5
		Milk C18_2c9t11 (g/dL)	0.00	0.14	0.03	0.02	0.74	37%	1.95	6
		Milk C18_3c9c12c15 (g/dL)	0.00	0.09	0.02	0.01	0.68	22%	1.77	5
		Milk Tot18_1cis (g/dL)	0.09	2.77	0.82	0.31	0.95	8%	4.58	2
		Milk Tot18_2 (g/dL)	0.01	0.32	0.10	0.03	0.69	15%	1.79	5
		Milk Total_C18_1 (g/dL)	0.10	2.98	0.94	0.33	0.96	7%	5.18	2
		Tot18_1trans (g/dL)	0.01	0.57	0.13	0.06	0.79	21%	2.17	4
		Milk Total_Trans (g/dL)	0.02	0.75	0.16	0.08	0.80	19%	2.26	4
		Milk isoanteiso FA (g/dL)	0.02	0.28	0.09	0.03	0.75	14%	2.00	5
		Milk Odd fatty acids (g/dL)	0.03	0.50	0.16	0.04	0.83	10%	2.41	4
		Milk omega3 (g/dL)	0.00	0.11	0.03	0.01	0.66	22%	1.73	5
		Milk omega6 (g/dL)	0.01	0.33	0.10	0.03	0.72	14%	1.89	5
		Milk SAT FA(g/dL)	0.31	6.97	2.70	0.75	0.99	3%	10.22	1
		Milk UNSAT (g/dL)	0.14	3.86	1.25	0.39	0.97	5%	5.75	2
		Milk MONO FA (g/dL)	0.12	3.42	1.08	0.35	0.97	5%	5.83	2
		Milk PUFA (g/dL)	0.02	0.53	0.16	0.05	0.77	13%	2.10	4
		Milk SCFA (g/dL)	0.05	0.80	0.35	0.10	0.93	7%	3.88	3
		Milk LCFA (g/dL)	0.19	4.79	1.59	0.52	0.95	7%	4.52	2
		Milk MCFA (g/dL)	0.22	5.48	2.00	0.60	0.97	5%	5.53	2

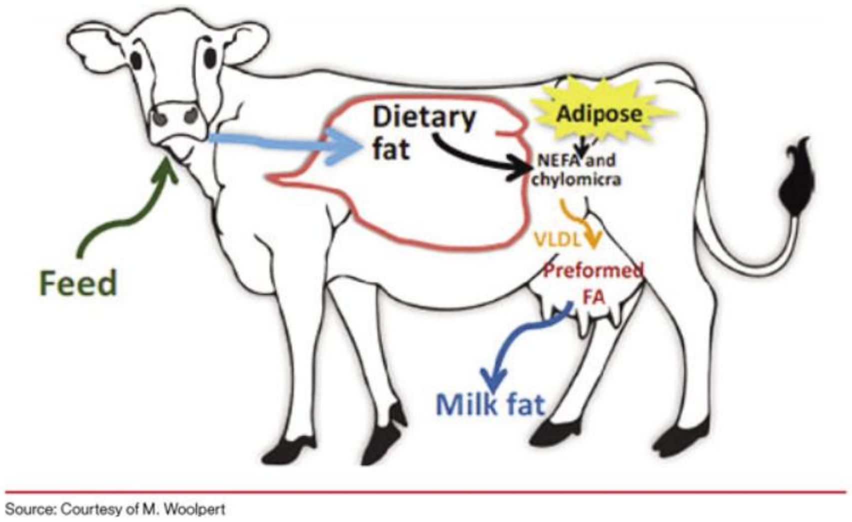
Fatty acids

De novo Fatty acids synthesis

Mixed and preformed Fatty acids synthesis

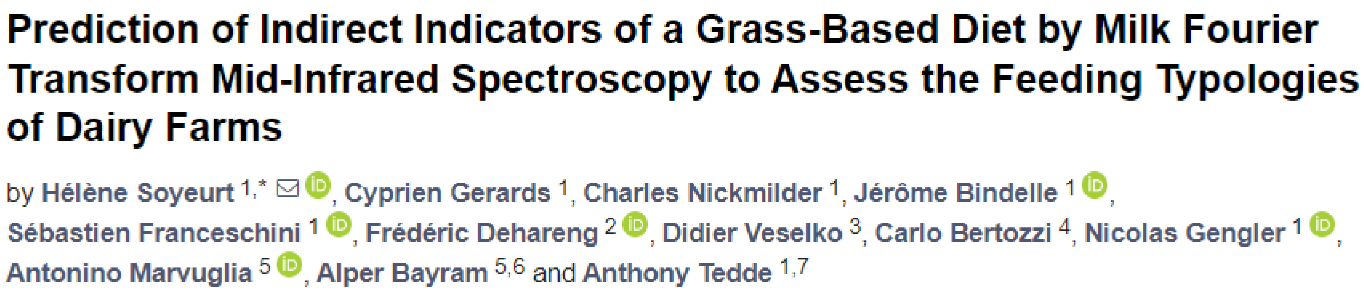
Rumination





Discrimination of the GRASS milk

Soyeurt et al., 2022

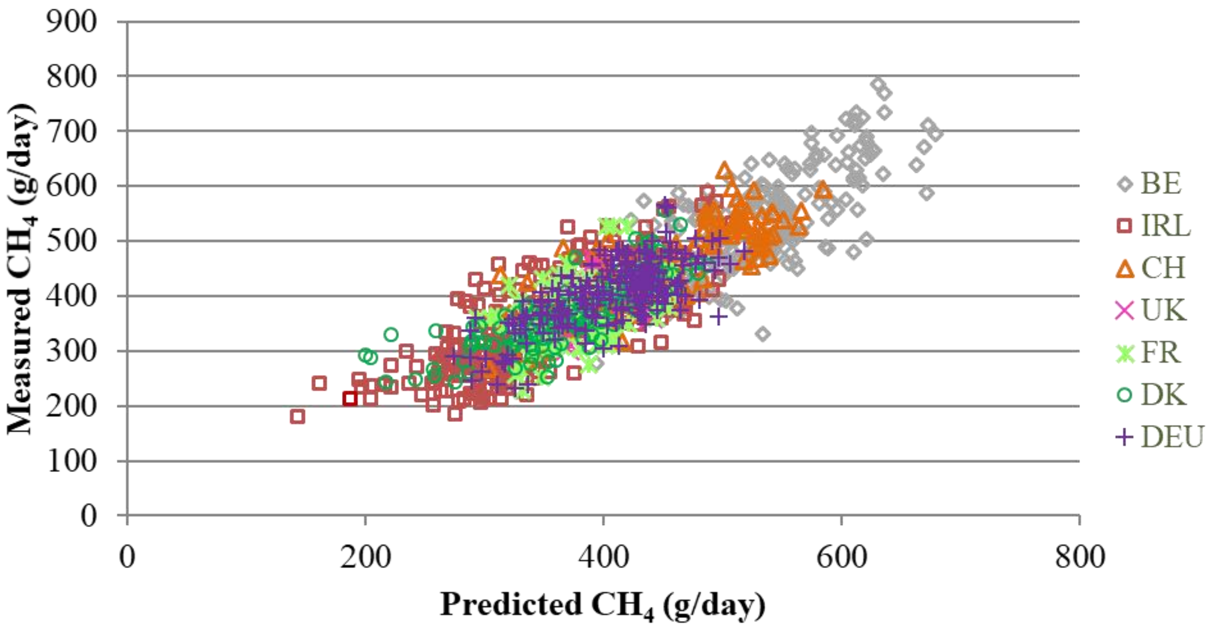

Prediction of Indirect Indicators of a Grass-Based Diet by Milk Fourier Transform Mid-Infrared Spectroscopy to Assess the Feeding Typologies of Dairy Farms

by Hélène Soyeurt [1,*], Cyprien Gerards [1], Charles Nickmilder [1], Jérôme Bindelle [1], Sébastien Franceschini [1], Frédéric Dehareng [2], Didier Veselko [3], Carlo Bertozzi [4], Nicolas Gengler [1], Antonino Marvuglia [5], Alper Bayram [5,6] and Anthony Tedde [1,7]

Indirect models e.g.: Methane emission, Health Status, Nitrogen Efficiency, Animal Stress, …

- Reference → Chambers, SF6, GreenFeed (Vanlierde et al., 2021)

Eructed methane

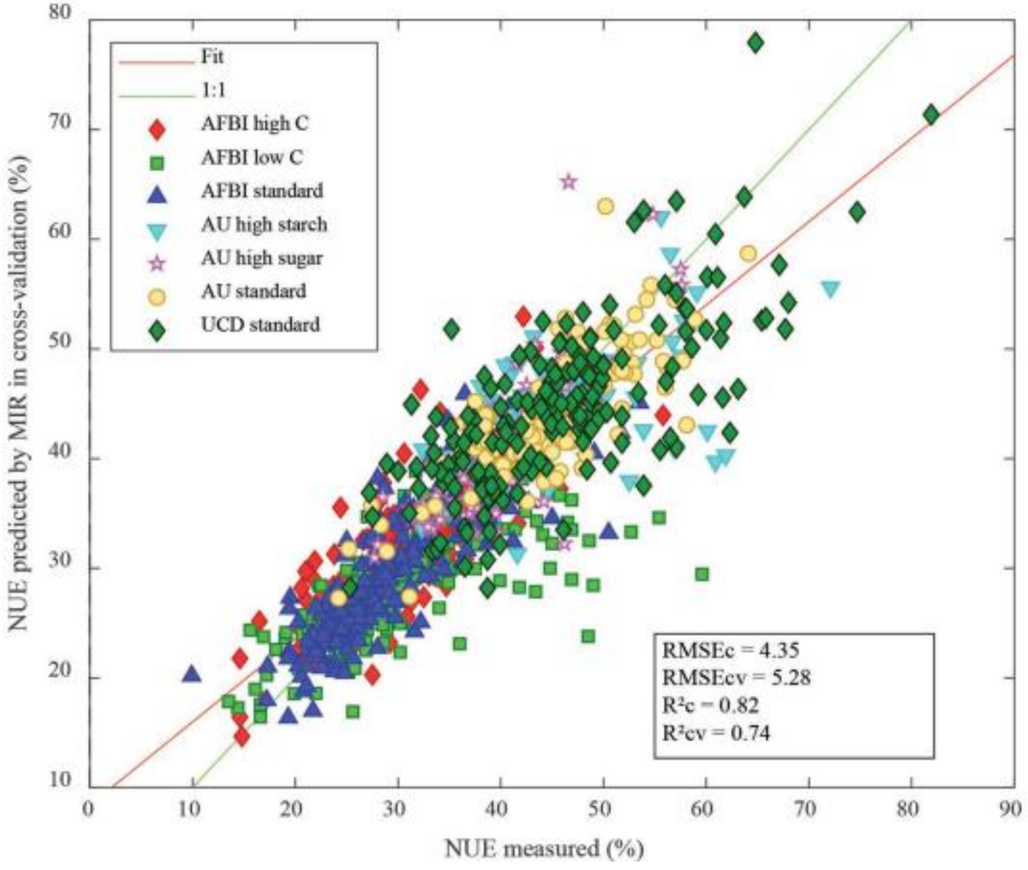


Groups of models		Predicted variable	Min	Max	Mean	SD	R^2cv	Relative RMSEcv	RPDcv	Model quality
CH4	CRA-W, Ulg, Teagasc, AFBI, INRA, DLQ, Aarhus, ETH-Zurich	Methane emitted (g/d)	180	786	413	102	0.68	14%	1.79	5

Indirect models

e.g.: Methane emission, Health Status, Nitrogen Efficiency, Animal Stress, …

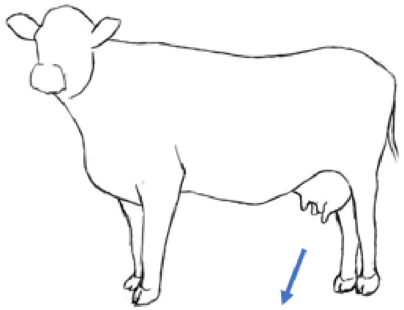
Nitrogen use efficiency (NUE)



Grelet et al., J. Dairy Sci. 103:4435–4445 (2020)

$$\text{N Use Efficiency (\%)} = \frac{\textit{N Out Milk}}{\textit{N Intake}} *100$$

N Intake (recorded daily)



N Out Milk (recorded twice weekly)

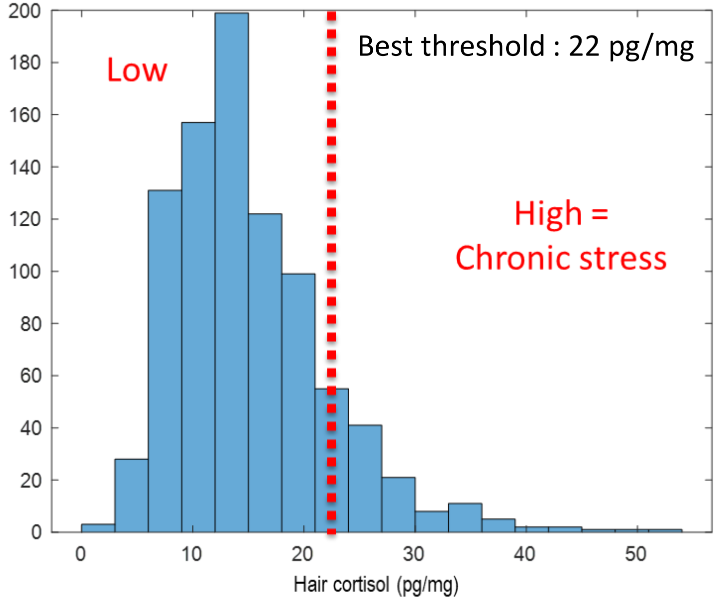
Model quality
5

Indirect models e.g.: Methane emission, Health Status, Nitrogen Efficiency, Animal Stress, …

Chronic stress

Cortisol discriminant models

Hair cortisol



Cross validation

	Low cortisol	High cortisol	
Predicted Low	719	73	
Predicted High	172	107	
	891	**180**	**1071**

Sensibility	Specificity	Accuracy
59.4%	81%	77%

External-Herd-Validation

	Low cortisol	High cortisol	
Predicted Low	656	71	
Predicted High	235	109	
	891	**180**	**1071**

Sensibility	Specificity	Accuracy
60.6%	74%	71%

Indirect models e.g.: Methane emission, Health Status, Nitrogen Efficiency, Animal Stress, …

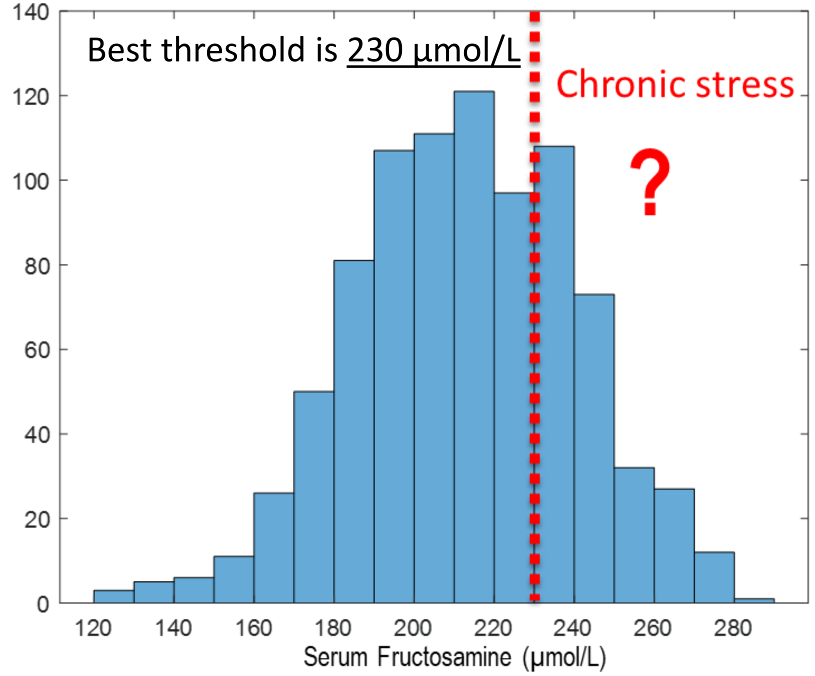
Chronic stress

Best model is with MIR only

Cross validation

	Low fructosamine	High fructosamine		Sensibility	Specificity	Accuracy
Predicted Low	513	58			75%	75%
Predicted High	175	194		77.0%		
	688	**252**	**940**			

Blood fructosamine



External-Herd-Validation

	Low fructosamine	High fructosamine		Sensibility	Specificity	Accuracy
Predicted Low	467	77			67.9%	68.3%
Predicted High	221	175		69.4%		
	688	**252**	**940**			

Pseudo-direct models e.g. Minerals or compounds with very low concentrations <100 ppm or mg/kg

Minerals : Christophe et al., 2021

- Nutritional quality
- Technological properties (cheese process)
- Cow status biomarkers (Mastitis…)
- Eutrophication issues

foods MDPI

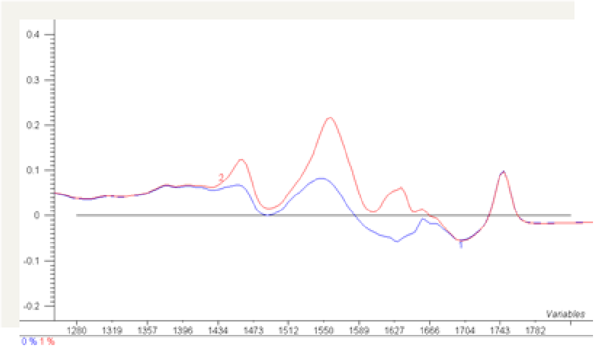
Article

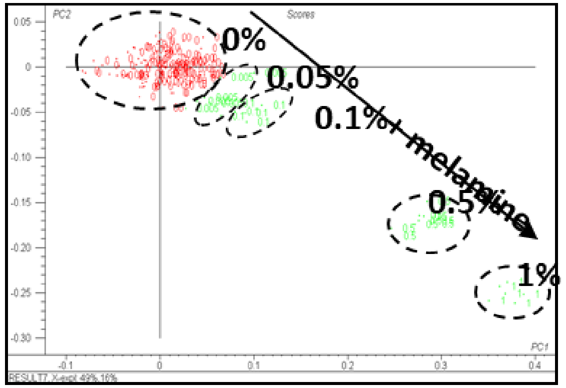
Multiple Breeds and Countries' Predictions of Mineral Contents in Milk from Milk Mid-Infrared Spectrometry

Octave S. Christophe [1], Clément Grelet [1], Carlo Bertozzi [2], Didier Veselko [3], Christophe Lecomte [4], Peter Höeckels [5], Andreas Werner [6], Franz-Josef Auer [7], Nicolas Gengler [8], Frédéric Dehareng [1,*] and Hélène Soyeurt [8]

Groups of models		Predicted variable	Min	Max	Mean	SD	R^2cv	Relative RMSEcv	RPDcv	Model quality
Milk minerals	CRA-W, Ulg, Teagasc, SRUC, FCEL, LKV-BW, LKV-NRW, LUKE, Valio, LKV-Austria	Milk Calcium (mg/kg)	593	1743	1149	135	0.82	5%	2.34	4
		Milk Magnesium (mg/kg)	61	157	100	13	0.72	7%	1.88	5
		Milk Sodium (mg/kg)	234	1273	356	91	0.44	15%	1.34	7
		Milk Phosphorus (mg/kg)	509	1447	999	124	0.75	6%	1.99	5
		Milk Potassium (mg/kg)	819	1985	1524	147	0.55	6%	1.48	5

Others models





ELSEVIER

Chemometrics and Intelligent Laboratory Systems

Volume 152, 15 March 2016, Pages 157-162

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 ☆

J.A. Fernández Pierna, D. Vincke, V. Baeten, C. Grelet, F. Dehareng, P. Dardenne

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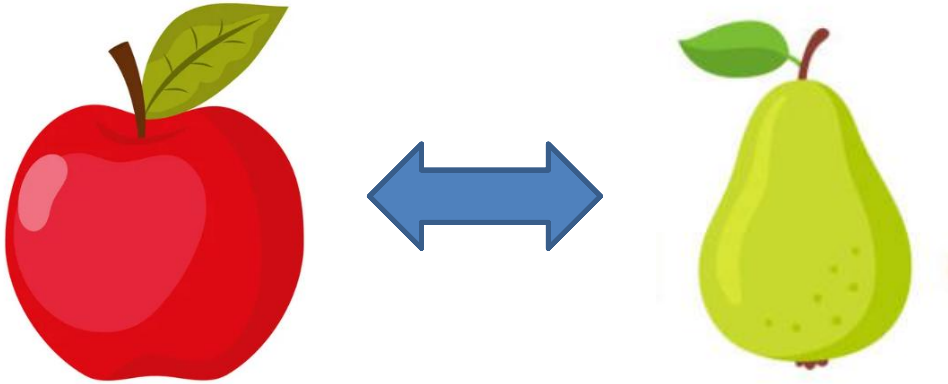
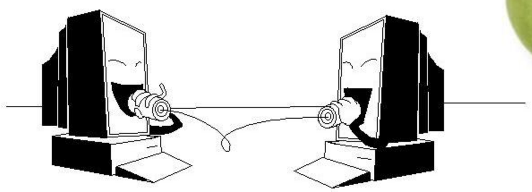
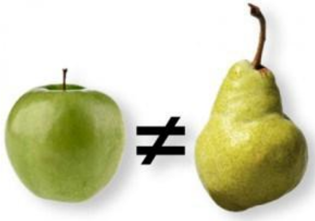


Objective and importance of MIR spectral standardization

Harmonization of spectra across instruments, labs, countries, continents

- Sharing of model
- Sharing of data (costly reference)


Harmonization of spectra across time

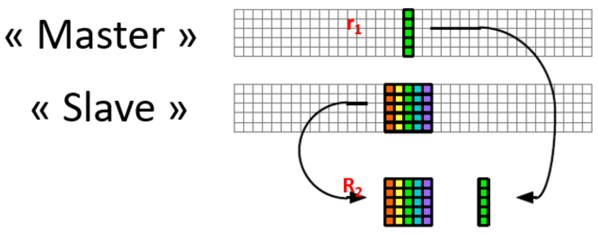
- Useability of models in time
- Stability of predictions

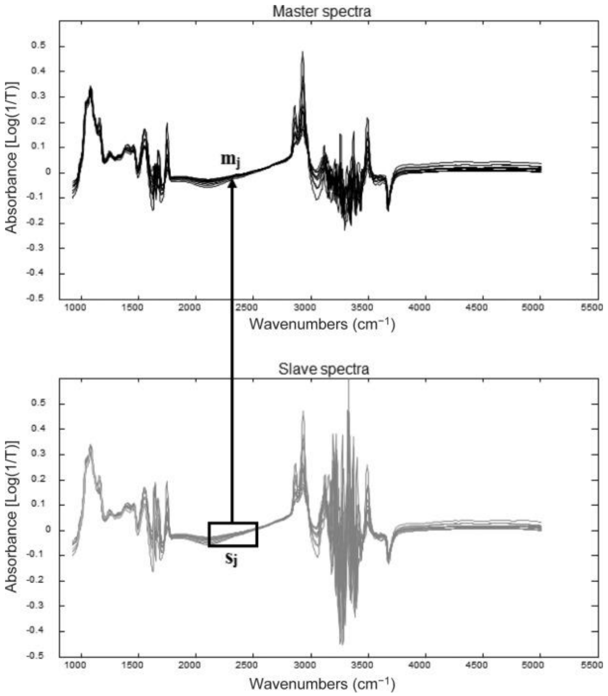
Harmonization of historical database

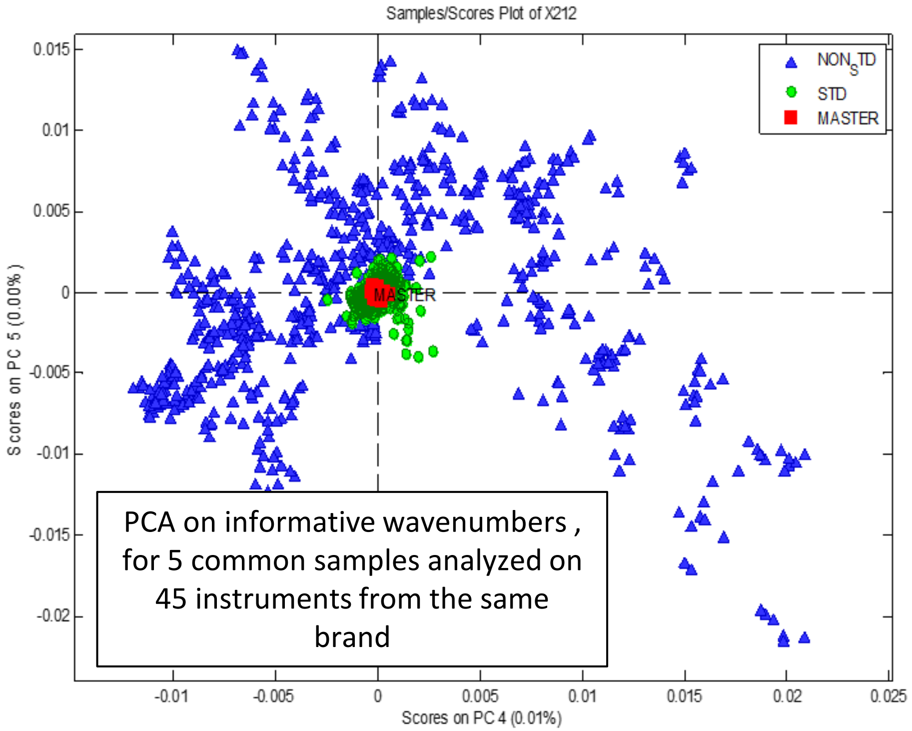
- Use of new models on historical spectra
- Power of big data
- Genetic evaluation

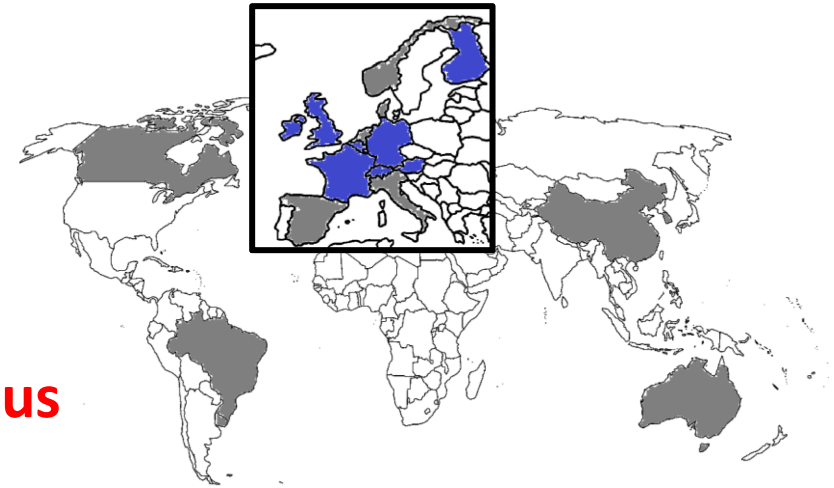
Standardization of MIR instruments

PIECE-WISE DIRECT STANDARDIZATION (PDS)









37 Labs
112 Apparatus

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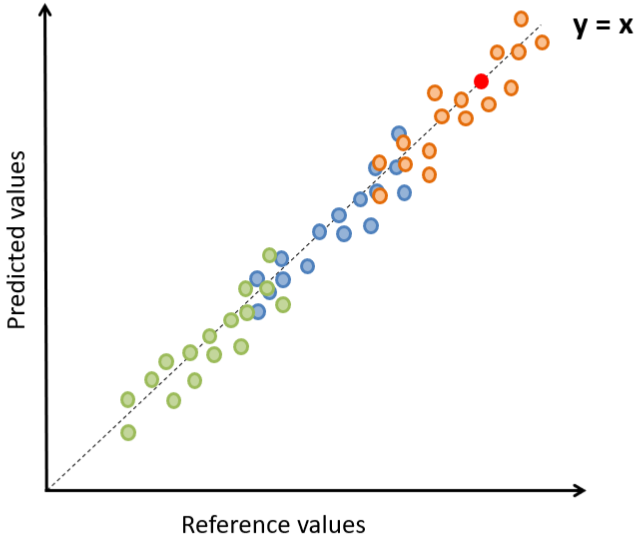

A lot of national & international collaborations

Wallonie recherche CRA-W
LIÈGE université Gembloux Agro-Bio Tech
INRAE
WAGENINGEN UNIVERSITY & RESEARCH
FRANCE CONSEIL ÉLEVAGE Donner du sens à la mesure
ZuchtData EDV-DIENSTLEISTUNGEN GMBH
EMR
EAAP European Federation of Animal Science
CONVIS LUXEMBOURG
awé GROUPE
ETH zürich
CdL comité du lait
Seenovia
teagasc Agriculture and Food Development Authority
GHENT UNIVERSITY
RVC Royal Veterinary College University of London
AARHUS UNIVERSITET
icbf
CRA Consiglio per la ricerca e la sperimentazione in agricoltura
afbi Agri-Food and Biosciences Institute
FBN
UCD DUBLIN University College Dublin An Coláiste Ollscoile, Baile Átha Cliath
Terre de fromages
QUALITAS
ELIANCE
CONSEIL ÉLEVAGE 25-90
Lactanet
dNmark research alliance
ICAR
SRUC
INSTITUT DE L'ELEVAGE idele
EFFAB European Forum of Farm Animal Breeders
LKV Baden-Württemberg
LKV
Huazhong Agricultural University
ISO
BOKU Universität für Bodenkultur Wien
eralytics
CyRIC
TU WIEN
NeoSpectra by Si-Ware
nanoplus
Université Gustave Eiffel
senseen
VIGO PHOTONICS
NMR information partnerships

Creation of historical spectral Database

Since 2008

Wallonie

Futurospectre DB

≈ 7.000.000 individual spectra

≈ 5.750.000 bulk spectra

Since 2023

Interreg Co-funded by the European Union

North-West Europe

HoliCow

HOLICOW

North-West Europe

≈ 60.000.000 individual spectra

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3 current areas of research :

Wallesmart, Holicow & Decide

To design and develop an innovative, interoperable, and collaborative digital platform tailored for livestock farming.

Its goal is to establish a network for gathering farm data from diverse stakeholders and collectively processing it to derive maximum actionable insights for decision-making.

Enable small and medium dairy farms to benefit from big data for holistic decision-making.

1. Health/welfare 2. Transformation 3. Fertility 4. Production 5. Environment 6. Heat Stress

Life cycle assessment is used to evaluate farm carbon footprint, ammonia emissions, and energy consumption. These are reported per unit of production or per hectare, considering both direct and indirect emissions.

Thanks to the 'DECiDE+ project', it's now available for dairy ewes and includes new environmental indicators such as N balance at farm level, feed autonomy, agroecological infrastructure importance, and indicators for economic and soon social dimensions to better assess overall farm sustainability, incorporating farming practices and agricultural features.

Wallonie recherche CRA-W

Thanks for your attention !

How mid-infrared spectroscopy of milk could contribute to improve the sustainability of the dairy sector

Frédéric Dehareng[1], Clément Grelet[1] & Amélie Vanlierde[2]

[1]*Quality and authentication of agricultural products Unit, CRA-W*
[2]*Animal production Unit, CRA-W*

IDF BENC Event, Connection and Interaction between Research and Practice, 18th April 2024