Webinar

Fatty Acids ExtraMIR project

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28th March 2023

Milk Analysis

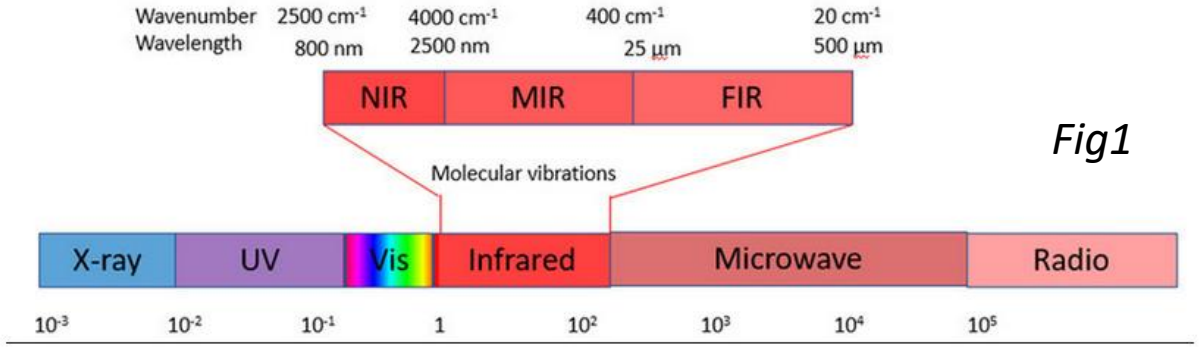
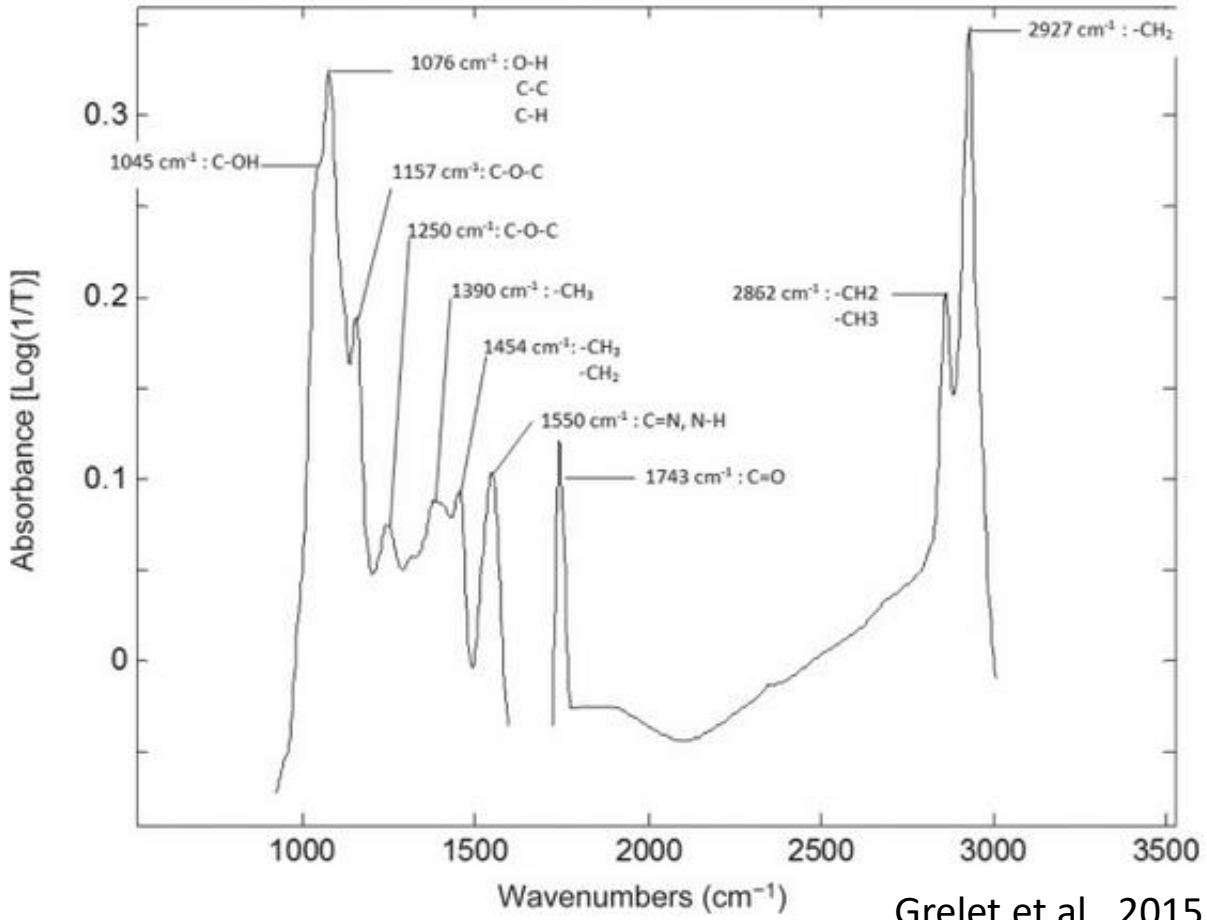


Fig1

Milk MIR spectrum
=
Absorption of infrared ray at frequencies related to the vibrations of specific chemical bounds in milk



Soyeurt, 2023

Grelet et al., 2015

What exists ?

Nutritional quality

Fat, protein, lactose, fatty acids, Ca, lactoferrin,…

Technological properties

Cheese yield, yoghurt yield, butter yield, spreadability …

Animal Health

Na, lactoferrin, Energy balance, body weight, dry matter intake, acetone, BHB, citrate …

Environmental fingerprint

Methane, P, urea …

Sustainability

Consumption index, nitrogen efficiency …

Abnormal milk samples, color …

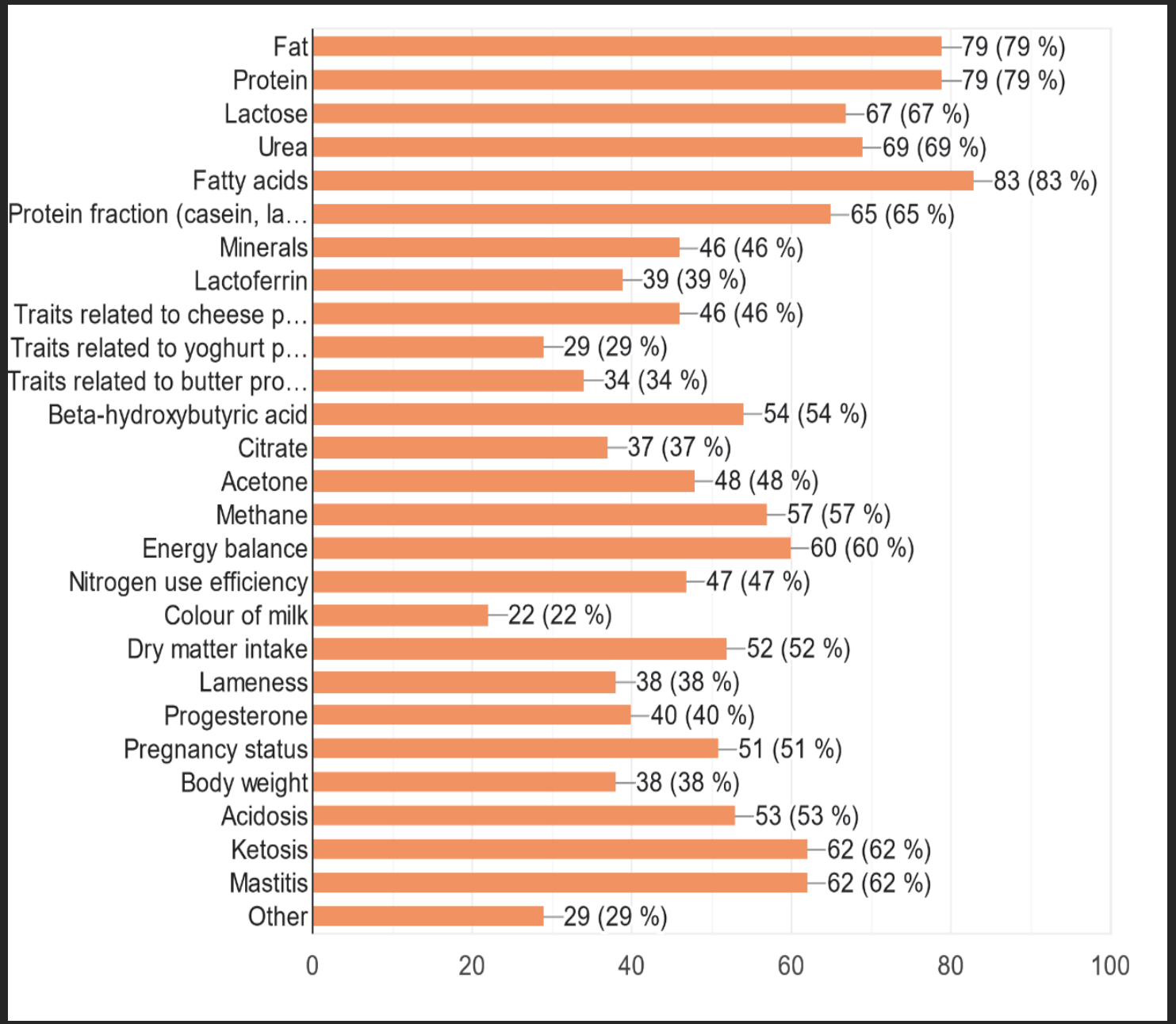
Soyeurt, 2023

Many research developments BUT ….

Limited applications on field at herd and (a little bit less for) individuals …

ExtraMIR

- ExtraMIR (**Extra** value from- smart use of -**MIR** spectra)
- Strong need for harmonization and standardization of terminology, analytical procedures, and tools for quality assurance.
- The entire dairy food chain is affected by these technological developments, IDF and ICAR are joining in structuring the current activity, offering a forum for exchange and cooperation, and harmonizing and standardizing definitions, methods, and procedures for the dairy sector globally.



Why Fatty Acids ?

- 106 respondents
- 59.4% want to actively participate in the project

Milk - Fatty acids

- Milk is a natural emulsion of fat suspended in water (= fat globules)
- The nucleus of those fat globules is composed of triglycerides
  (98 to 99% of the fat in milk)
- Triglyceride = glycerol + fatty acids

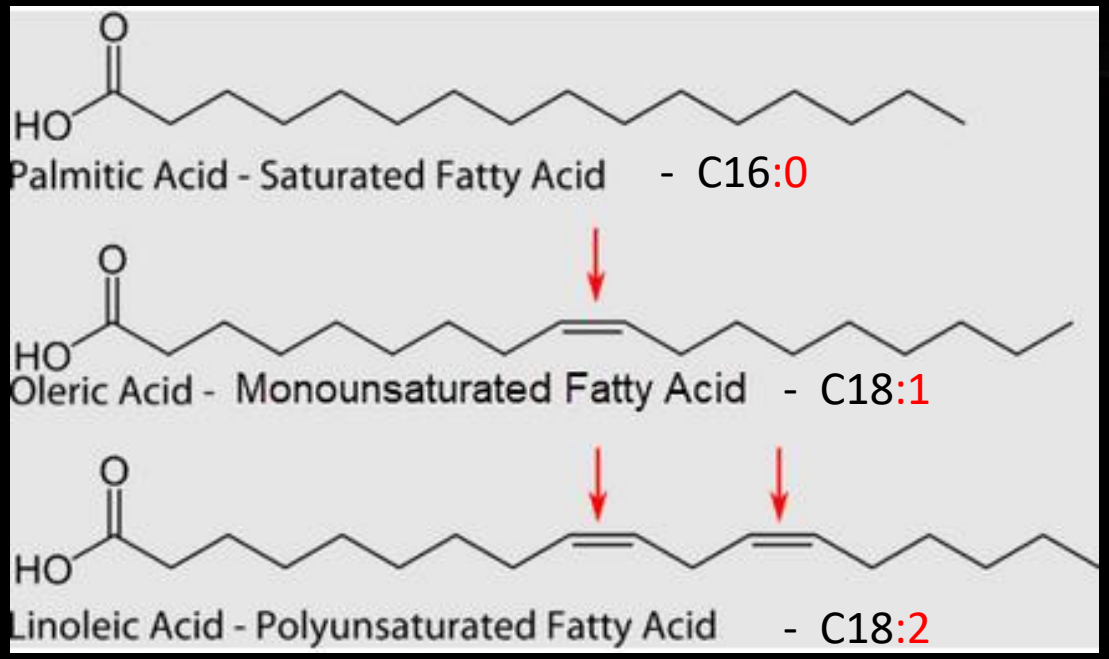
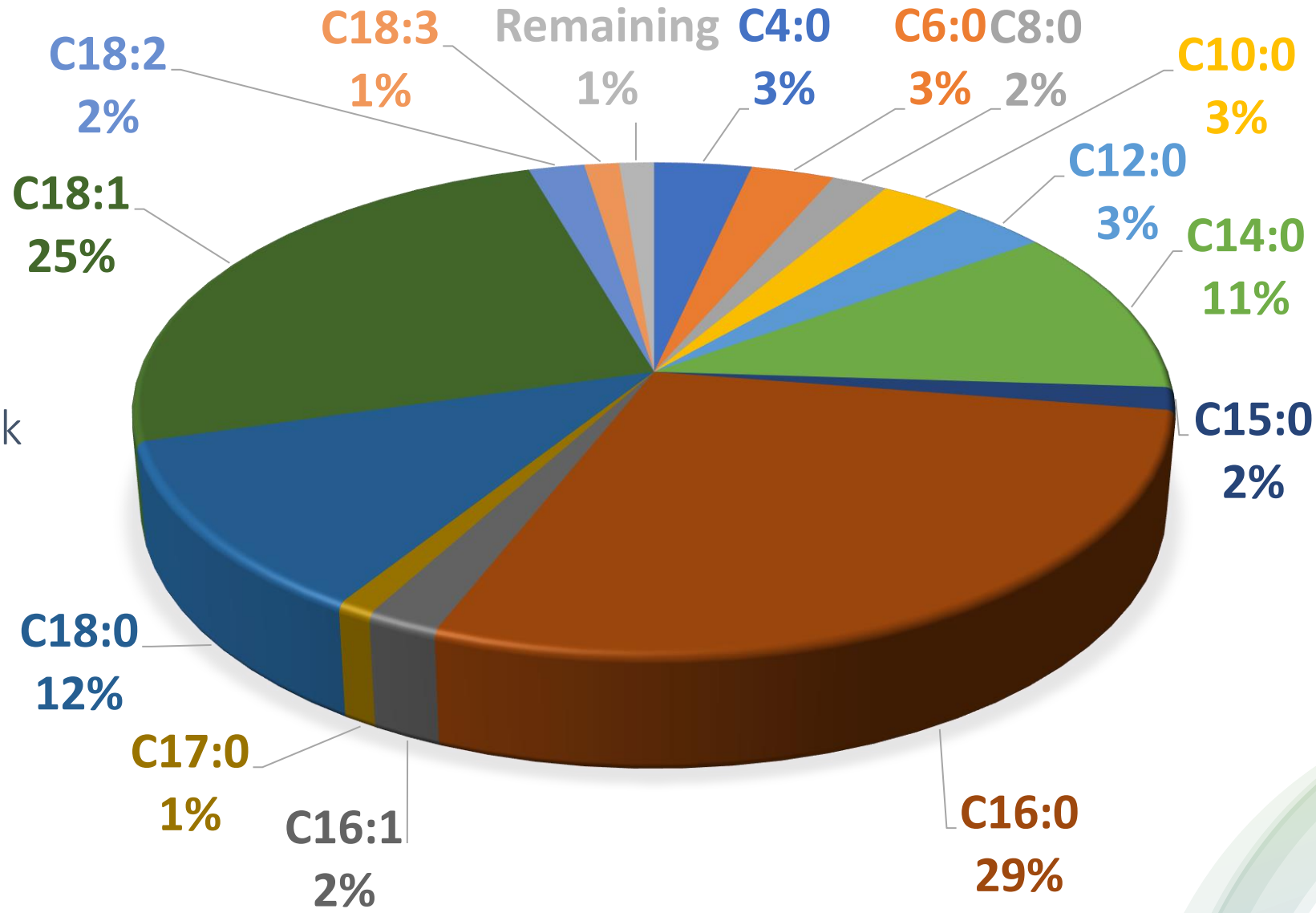


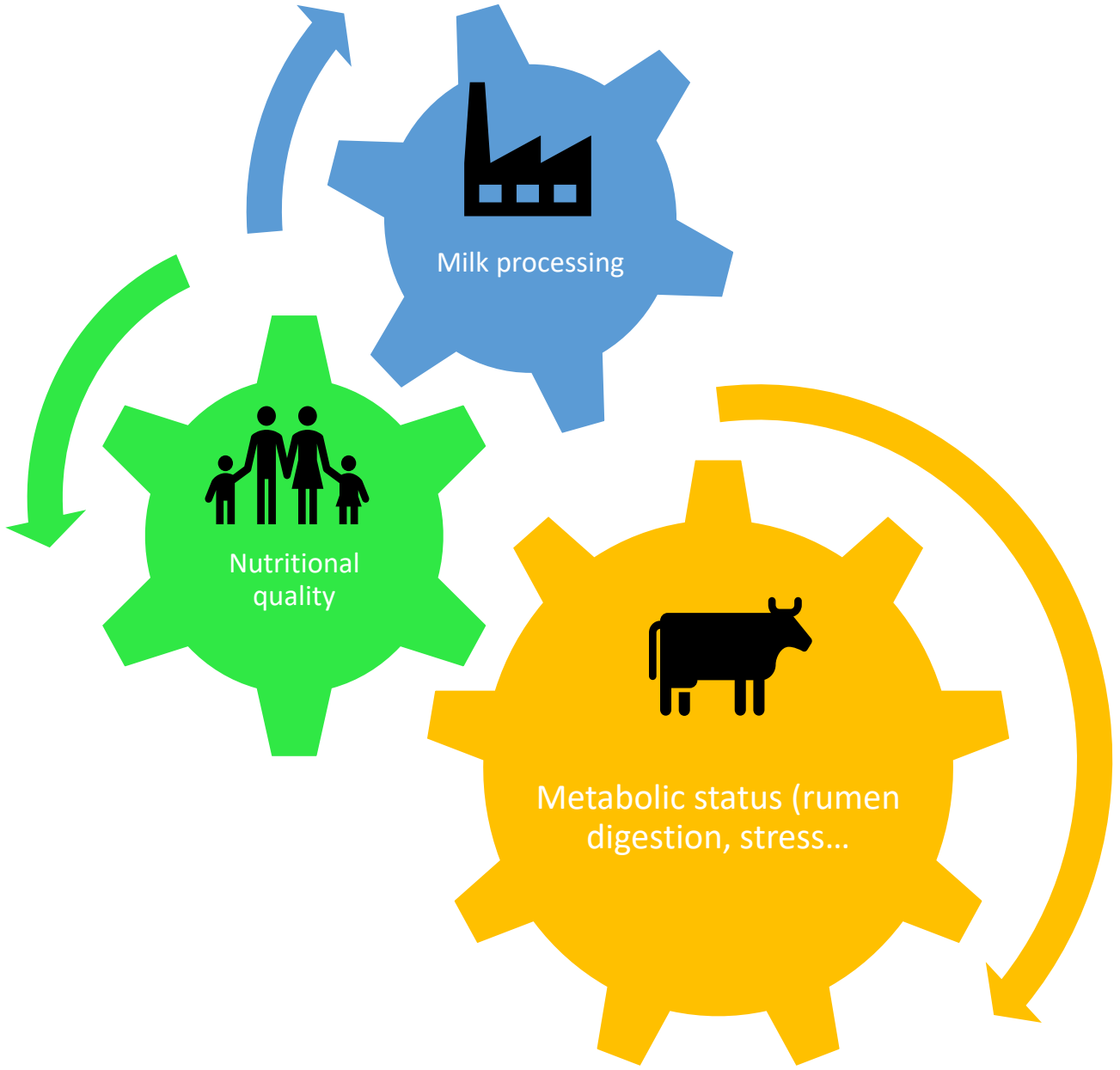
Fig1

Up to 400 fatty acids in milk
but
Few are mainly present



- Adapted from Gervais et al. (2017)

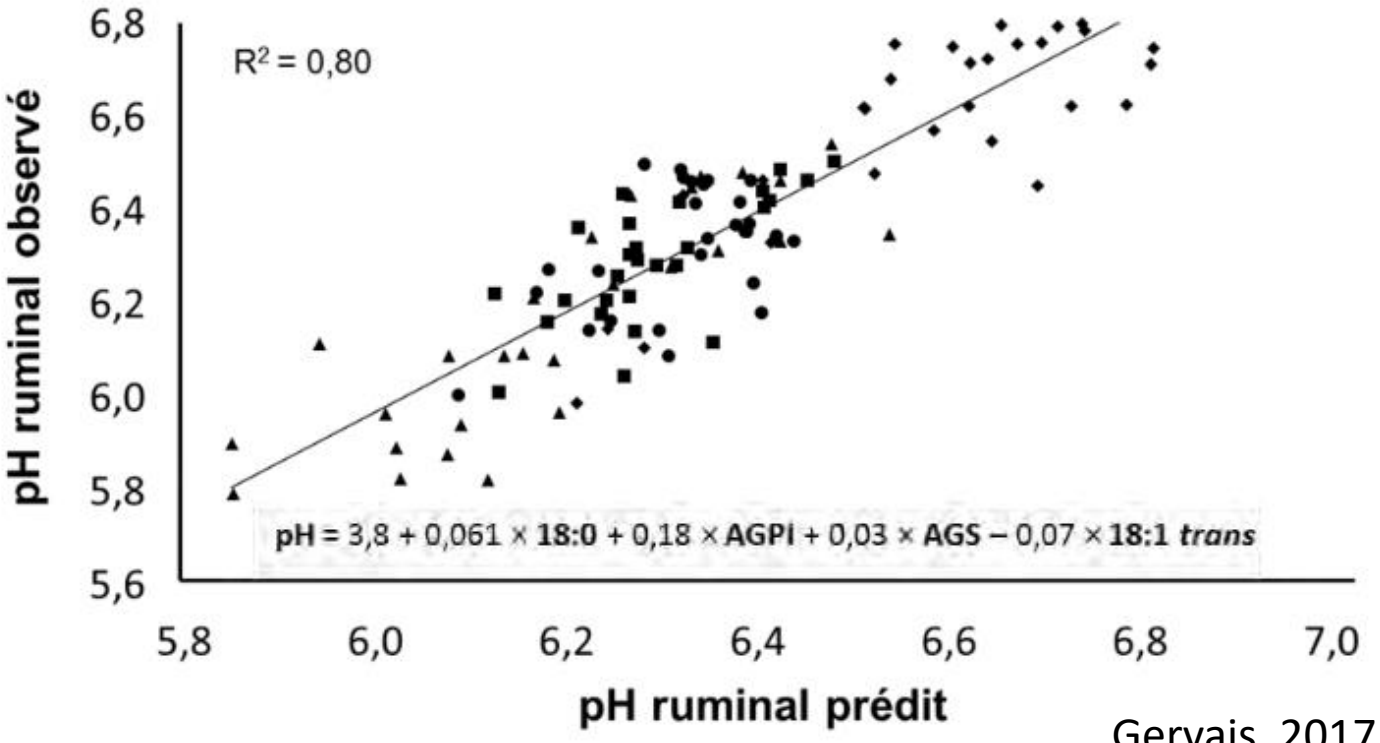
Interests


Milk processing
Nutritional quality
Metabolic status (rumen digestion, stress…

Cow level

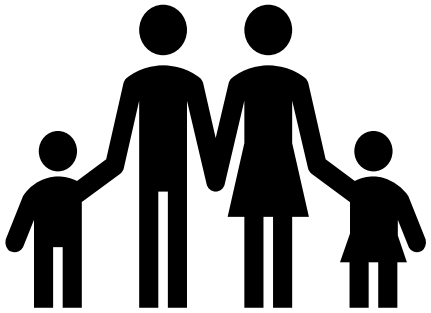
- Knowing the FA composition is interesting for :
  - the efficiency of ruminal fermentation,
  - The metabolic health of the cow (e.g. energy deficit)
  - The quantification of enteric methane emissions

pH ruminal using FT-MIR FA predictions



Gervais, 2017

pH = 3.8 + 0.061 x C18:0 + 0,18 x PUFA + 0.03 x SFA x trans C18:1



Society level

Milk is one of the most consumed food in the world

Nutritional quality

Health index

=

UFA / (C12:0 + C14:0 x 4 + C16:0)

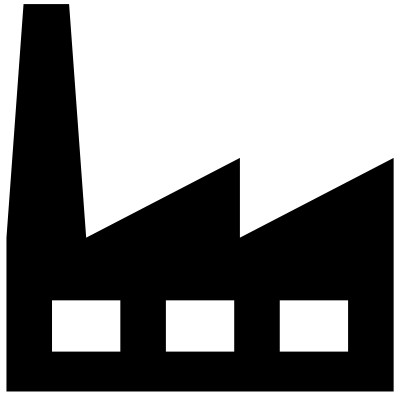
Fatty acids are not harmful to human health, but their excess in the daily diet, yes.

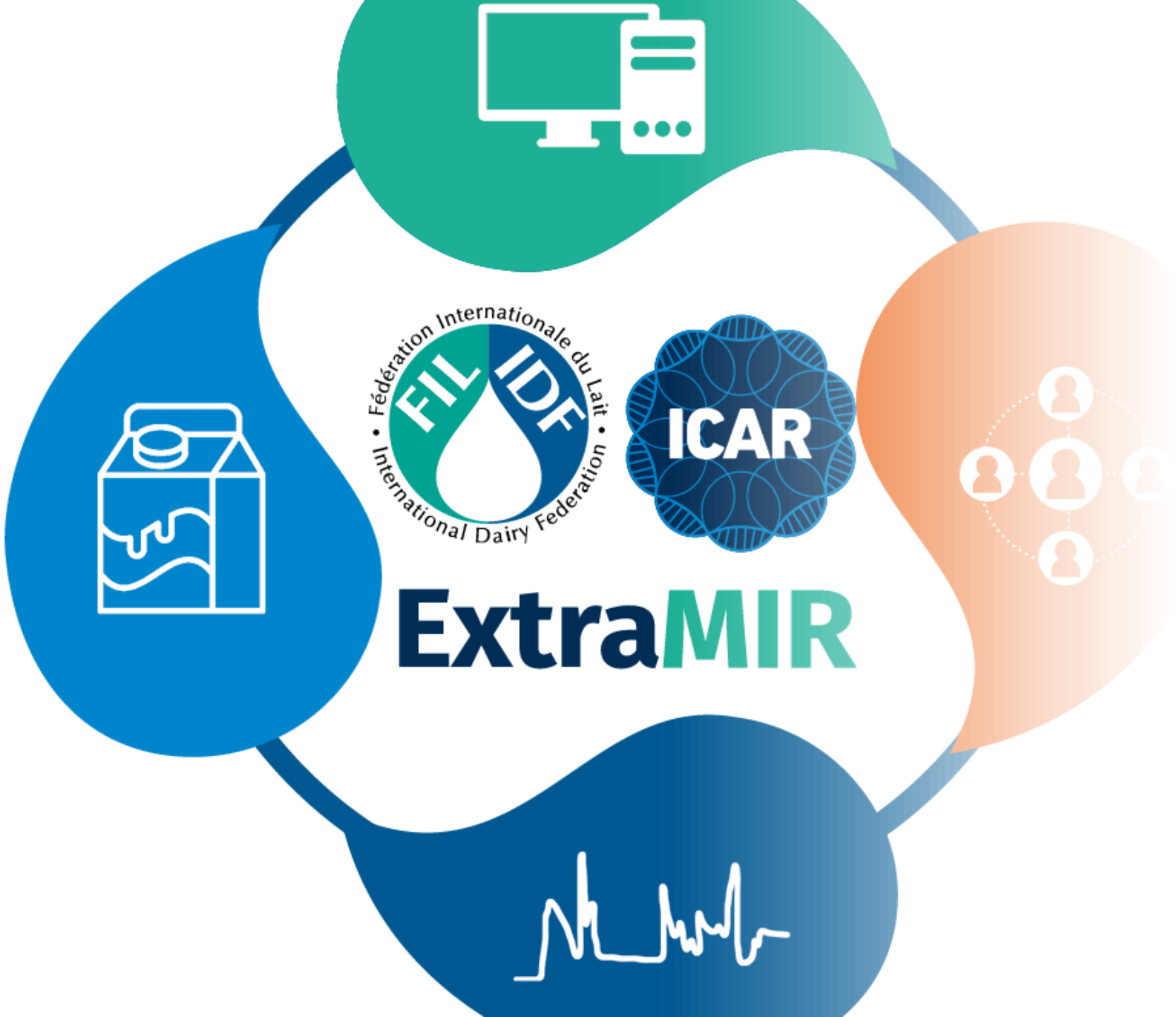
Following “Institut de l’Elevage”, the aimed milk composition should be :

less rich in saturated FA (around 60 to 65%) with less palmitic acid (C16:0)	richer in omega3 FAs	the maintenance or even a slight decrease in the content of omega6 and of some trans FA (C18:1 t9 and t10)	a ratio omega6/omega3 lower than 5 (recommendation of the Anses)	a good rumenic acid content (CLA c9t11)

Industry interest

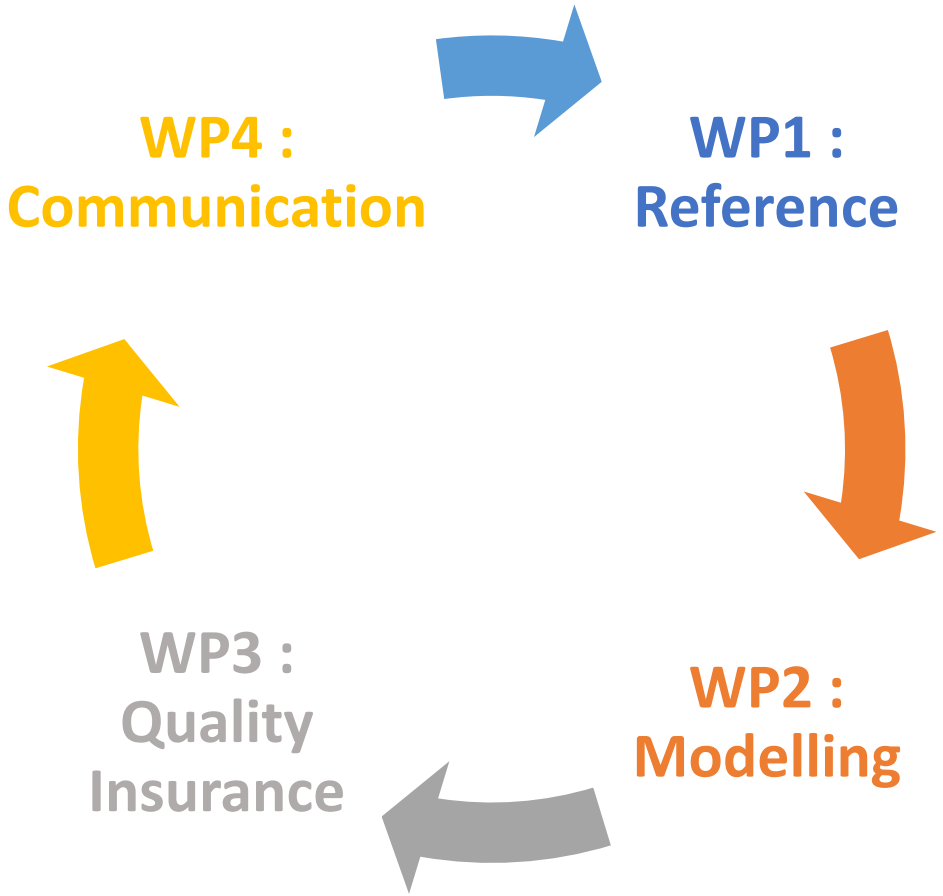
- Cow’s well being linked to previous slides
- Butter spreadability
  - Higher value for C18:1 cis-9 / C16
- Methane emission (even if direct equation exists)





Fatty Acids
ExtraMIR project

4 Work packages



We have started to work …

- **2022-2023 Brian Wickham Young Persons Exchange Program Bursaries Awards**
- Michael Whittaker
  - Cattle Information Systems, UK
  - ICAR Milk Analysis Sub-Committee and having Christian Baumgartner as Chair

Travels in :

- Belgium
- New-Zealand
- Canada

4 Work packages

- List potential contributors
- Compare reference analytical methods
- Standardize the methods or define a correction

WP1 : Reference

WP2 : Modelling

- List potential contributors
- Create a common validation set
- Create a tool to compare the prediction performances

Fatty acids Equations

- At least 11 teams
  - 8 from the scientific community
  - 3 from spectrometer providers

Different accuracy

RPDcv	Relative RMSEcv	R^2cv	Interpretation for application
> 6	<5%	> 0.97	Any application (e.g., Saturated FA, Monounsaturated FA,…)
4.2 - 6	<10%	0.94 - 0.97	Quality control (e.g. Medium-chain FA, C18:1 cis-9, Long chain FA …)
3 - 4.2	<10%	0.89 - 0.94	Quantitative screening (e.g. , C14:0, C4:0, C6:0)
2 - 3	<25%	0.74 - 0.89	Rough screening (e.g. Polyunsaturated FA, C17:0 …)
1.5 - 2	<25%	0.55 - 0.74	Allows to compare groups, discriminate high or low values (e.g., C16:1 cis-9…)
1.5 -2	>25%	0.55 - 0.74	Highly imprecise, can be used to detect extreme values (e.g., C18:3 cis-9,cis-12,cis-15)
< 1.5	-	< 0.55	Not recommended

Need to compare the validation results on a same basis to have a more precise prediction error

ExtraMIR tool under construction …
➔ collaboration development

ExtraMIR tool

Enter the date using the format YYYY-MM-DD

Enter your institution name

Spectra Download | Data upload | Data check | Prediction statistics | Spectral representativity | Validation performances | Report download | Data sharing agreement

Download the validation milk MIR spectra

Download

sampleID	X1	X2	X3	X4	X5	X6	X7	X8	X9	X10	X11	X12	X13	X14	X15
144	-0.08	-0.08	-0.08	-0.07	-0.07	-0.07	-0.06	-0.06	-0.06	-0.05	-0.05	-0.04	-0.03	-0.02	-0.01
145	-0.07	-0.07	-0.07	-0.06	-0.06	-0.06	-0.06	-0.05	-0.05	-0.05	-0.04	-0.04	-0.03	-0.02	-0.00
146	-0.08	-0.08	-0.07	-0.07	-0.07	-0.06	-0.06	-0.06	-0.06	-0.05	-0.05	-0.04	-0.03	-0.02	-0.01
147	-0.07	-0.06	-0.06	-0.06	-0.06	-0.05	-0.05	-0.05	-0.05	-0.04	-0.04	-0.03	-0.02	-0.01	-0.00
148	-0.08	-0.07	-0.07	-0.07	-0.06	-0.06	-0.06	-0.06	-0.05	-0.05	-0.04	-0.04	-0.03	-0.02	-0.00
149	-0.07	-0.07	-0.07	-0.06	-0.06	-0.06	-0.06	-0.05	-0.05	-0.05	-0.04	-0.04	-0.03	-0.02	-0.00

ExtraMIR tool under construction …
➔ collaboration development

Validation performances from the entire dataset - data view

	RMSE	MAE	R2	MeanPred	MeanRef	SdPred	SdRef	MinPred	MinRef
C4	0.013	0.101	0.788	0.102	0.111	0.018	0.021	0.062	0.063
C6	0.009	0.089	0.850	0.070	0.077	0.015	0.016	0.041	0.041
C8	0.007	0.075	0.825	0.044	0.049	0.011	0.011	0.019	0.022
C10	0.011	0.098	0.921	0.102	0.109	0.030	0.031	0.033	0.037
C12	0.014	0.109	0.921	0.124	0.133	0.038	0.040	0.041	0.038
C14	0.037	0.175	0.921	0.420	0.443	0.104	0.101	0.228	0.215
C14_1	0.006	0.068	0.807	0.040	0.042	0.012	0.013	0.017	0.017
C16	0.059	0.222	0.958	1.077	1.064	0.281	0.282	0.597	0.541
C16_1c	0.009	0.083	0.799	0.066	0.065	0.018	0.019	0.035	0.037
C17	0.002	0.038	0.919	0.027	0.026	0.006	0.005	0.014	0.016
C18	0.050	0.203	0.816	0.366	0.358	0.104	0.116	0.149	0.135
totC18_1trans	0.027	0.152	0.702	0.121	0.126	0.045	0.049	0.016	0.033
C18_1cis9	0.078	0.260	0.902	0.731	0.693	0.210	0.219	0.295	0.218
toC18_1cis	0.048	0.202	0.956	0.787	0.776	0.221	0.225	0.325	0.284
C18_2	0.010	0.091	0.855	0.089	0.082	0.016	0.017	0.049	0.037
C18_2c9c12	0.010	0.093	0.467	0.054	0.051	0.009	0.014	0.035	0.018
C18_3c9c12c15	0.004	0.053	0.866	0.022	0.024	0.006	0.007	0.010	0.006
C18_2c9t11	0.009	0.085	0.755	0.035	0.040	0.014	0.014	0.008	0.009
SAT	0.091	0.283	0.981	2.489	2.535	0.569	0.555	1.471	1.537
MONO	0.043	0.190	0.980	1.054	1.038	0.281	0.275	0.434	0.397
POLY	0.015	0.111	0.888	0.158	0.165	0.039	0.040	0.068	0.056
INSAT	0.050	0.207	0.976	1.216	1.204	0.315	0.311	0.508	0.454
SCFA	0.044	0.192	0.869	0.324	0.359	0.074	0.077	0.178	0.185
MCFA	0.108	0.293	0.961	1.838	1.895	0.468	0.461	0.987	0.943
LCFA	0.110	0.299	0.939	1.531	1.483	0.397	0.401	0.628	0.537
isoanteiso	0.018	0.124	0.698	0.087	0.101	0.019	0.018	0.038	0.056
omega3	0.004	0.057	0.791	0.028	0.029	0.008	0.007	0.013	0.014
omega6	0.007	0.073	0.874	0.095	0.096	0.018	0.019	0.051	0.047

4 Work packages

WP1 : Reference

- List potential contributors
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WP2 : Modelling

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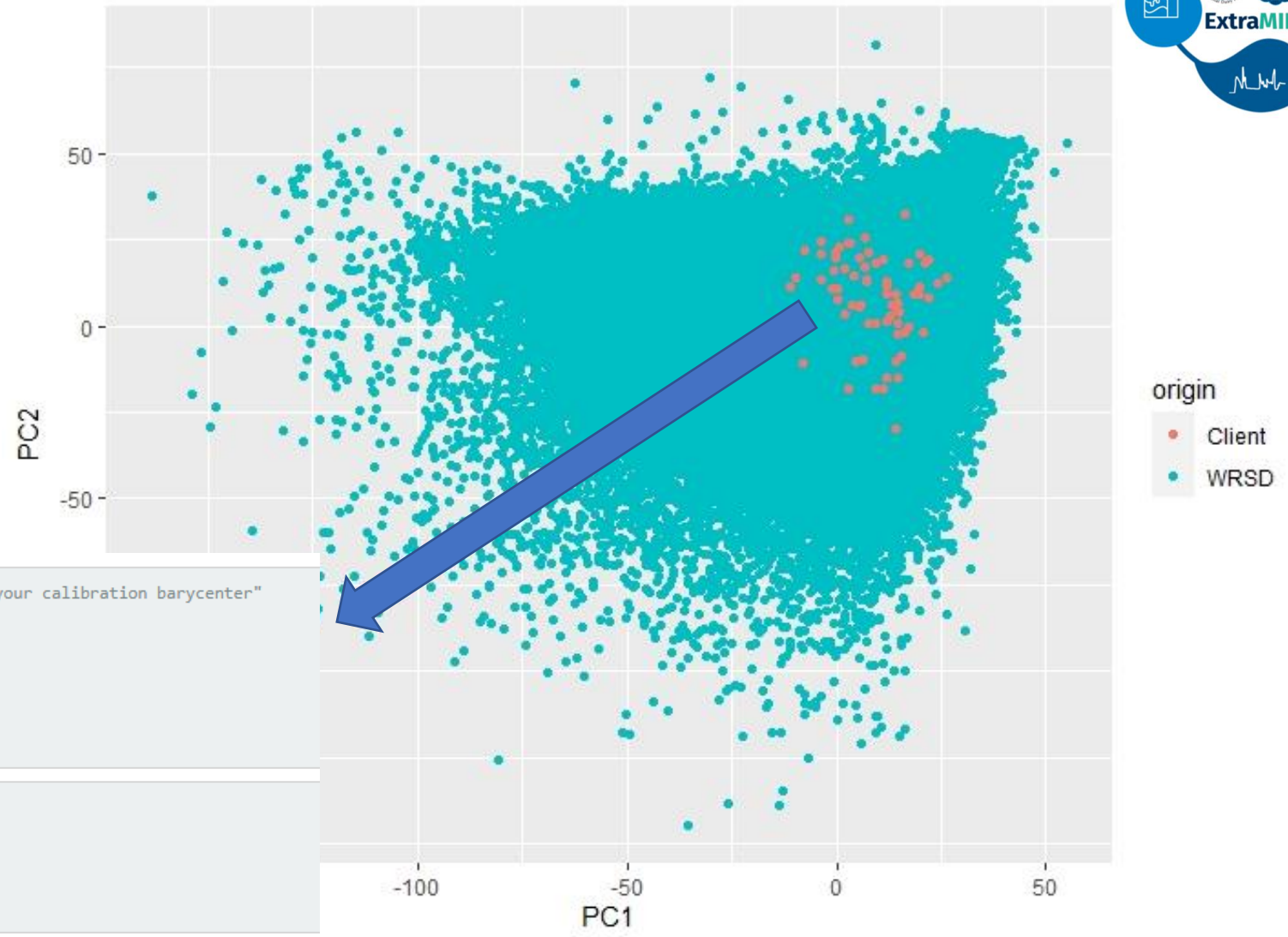
WP3 : Quality Insurance

- Compare the different spectral standardization
- Develop an approach to avoid spectral extrapolation when a FT-MIR prediction is made
- Create a World Representative Spectral Database (WRSD)
- Create a tool to define the part of the spectral variability covered by a calibration set

WP4 : Communication



Client = spectra from a calibration set

```
[1] "Distribution of WRSD samples following their Global-H (GH) distance from your calibration barycenter"

----------------------------------------
   0%      25%     50%     75%    100%
-------- ------- ------- ------- -------
 0.3009   2.676   3.976   6.384   166.2
----------------------------------------
```

```
[1] "The master spectra file contained 376939 spectra."
[1] "You have provided 71 spectra."
[1] "From your WRSD dataset, there were 120546 with a GH between 3 and 5."
[1] "There were 136536 with a GH higher than 5."
[1] "Your dataset covers 68.0197591652761% of spectral variability"
```

4 Work packages

- Propose a guideline to standardize the spectral data
- Propose a guideline to measure the FA contents in milk
- Propose a guideline to validate the FA equation
- Discuss the use of FA on field for dairy farmers and industry

WP4 : Communication

- List potential contributors
- Compare reference analytical methods
- Standardize the methods or define a correction

WP1 : Reference

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Collaborative learning

Organization

For the registered persons, you will receive soon an e-mail…

Action leader: **Hélène Soyeurt (BEL)**

WP1

- Proposed WP leader :
  - **Josée Bordeleau (CAN)**
- Participants
- Observers

WP2

- Proposed WP leader:
  - **Steve Holroyd (NZ)**
- Participants
- Observers

WP3

- Poposed WP leader:
  - **Frédéric Dehareng (BEL)**
- Participants
- Observers

WP4

- Proposed WP leader:
  - **Michael Whittaker (UK)**
- Participants
- Observers

For the registered persons, you will receive soon an e-mail…

You want to join the project ……..

Send an e-mail to

Anabel Mulet Cabero
FIL-IDF
amulet@fil-idf.org

Silvia Orlandini
ICAR
silvia@icar.org

Webinar

Fatty Acids ExtraMIR project

Hélène Soyeurt

hsoyeurt@uliege.be

28th March 2023

- Moderator: Rob Crawford (5min)
- Speaker 1: Christian – ExtraMIR – setting the scene for the joint IDF/ICAR project (5 min)
- Speaker 2: Steve – ExtraMIR - current applications and challenges along the dairy food chain (15 min)
- Speaker 3: Hélène – ExtraMIR - Fatty Acid Composition as first example for an ExtraMIR project (20 min)
- Q&A session (15 min)

- Milk bottle adapted from https://burst.shopify.com/photos/hand-holds-a-glass-bottle-of-milk
- Road picture : https://pantonium.com/wp-content/uploads/2020/06/matthew-henry-_XYtu0lcVWo-unsplash-scaled.jpg
- Fig1 : https://www.researchgate.net/figure/Spectral-range-for-near-infrared-NIR-and-mid-infrared-MIR-showing-wavelengths-nm_fig1_338633707
- Fig1 : https://chem.libretexts.org/Courses/University_of_Kentucky/UK%3A_CHE_103_-_Chemistry_for_Allied_Health_%28Soult%29/Chapters/Chapter_14%3A_Biological_Molecules/14.2%3A_Lipids_and_Triglycerides
- Gervais et al. 2017: https://www.agrireseau.net/documents/Document_99830.pdf
- Soyeurt, 2023 : https://www.sciencedirect.com/science/article/pii/S2666910222001570
- Grelet et al. , 2015 : https://www.sciencedirect.com/science/article/pii/S0022030215000910
- https://oxford-review.com/why-some-people-learn-better-using-cooperative-learning-techniques/