Creation of universal MIR calibrations by standardization of milk spectra: example of fatty acids

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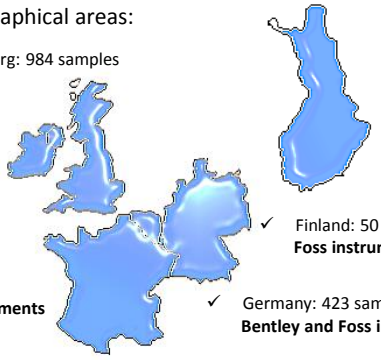
Context and objectives

- Fatty acid content of cow milk can be predicted by Mid-Infrared, however to build **robust** MIR equations, a **large spectral dataset** with samples covering the maximum chemical variability is needed
- The sharing of data is a potential solution, but due to the **differences existing between each MIR instruments**, a step of **spectral standardisation** is necessary
- Then the goal of this research is to bring the spectra from different types and brands of MIR instruments in the same format, by using a standardisation method, in order to build and use common MIR calibrations predicting fatty acids content of milk

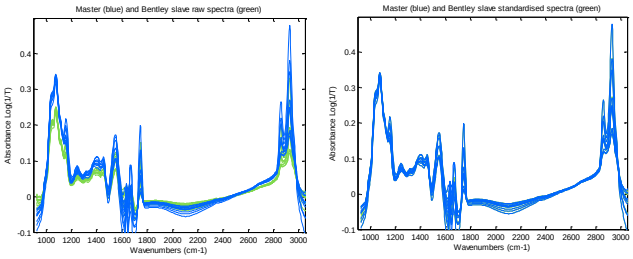
Fatty acids analysis and standardisation of MIR instruments

- **1827** milk samples selected on spectral variability and analyzed in MIR (2 brands, Foss and Bentley) and in GC to obtain fatty acid profile (since 2006).
- Dataset covering large variability of breeds (17), seasons, feeding systems and geographical areas:



- ✓ Belgium and Luxembourg: 984 samples **Foss instruments**
- ✓ UK: 106 samples **Foss instruments**
- ✓ Ireland: 144 samples **Foss instruments**
- ✓ France : 150 samples **Bentley and Foss instruments**
- ✓ Finland: 50 samples **Foss instruments**
- ✓ Germany: 423 samples **Bentley and Foss instruments**

- Method used: Piecewise Direct Standardisation
- Milk MIR spectra from all "slaves" instruments are mathematically corrected to be in the format of the "Master" instrument via analysis of common milk samples



- Partial Least Square method (PLS) used to build calibrations
- **1371** samples used as calibration dataset (including 66 Bentley)
- **456** samples used as validation dataset (including 22 Bentley)

Results and discussion

- Standardisation allows to bring all the spectra from different instruments into the "master" spectral format, and to group them into a common database
- Common FA equations where created for all instruments, including Foss and Bentley
- Validation results (with Foss and Bentley) are comparable to calibration results, showing good ability of the equations to be used on all instruments (even on Bentley standardized spectra)

Constituents (g/100 ml milk)	Calibration using 1371 samples # terms	Mean	SD	SEC	R^2c	Validation (456 samples) SEP	R^2p	RPDp	Use
Fat	7	3.906	0.981	0.007	1.00	0.007	1.00	140.11	+++
Total of Saturated FA	8	2.694	0.757	0.072	0.99	0.082	0.99	9.23	+++
Total of Mono-unsaturated FA	10	1.073	0.344	0.059	0.97	0.066	0.97	5.20	++
Total of Poly-unsaturated FA	11	0.159	0.045	0.021	0.79	0.023	0.75	1.97	-
Total of Unsaturated FA	10	1.233	0.379	0.064	0.97	0.076	0.96	4.99	+
Total of Short chain FA	9	0.348	0.097	0.025	0.93	0.027	0.92	3.59	+
Total of Mid chain FA	11	1.988	0.606	0.104	0.97	0.123	0.95	4.93	+
Total of Long chain FA	10	1.579	0.498	0.110	0.95	0.126	0.95	3.95	+
Total of branched FA	9	0.091	0.026	0.013	0.77	0.015	0.64	1.74	-
Total of odd FA	10	0.156	0.041	0.016	0.84	0.019	0.76	2.14	0
Total of trans FA	13	0.159	0.068	0.029	0.82	0.036	0.76	1.90	-
C4:0	11	0.104	0.029	0.008	0.93	0.009	0.90	3.21	+
C6:0	8	0.072	0.021	0.006	0.91	0.007	0.89	2.97	0
C8:0	9	0.047	0.014	0.004	0.91	0.005	0.88	2.78	0
C10:0	12	0.111	0.035	0.010	0.92	0.011	0.89	3.17	+
C12:0	12	0.134	0.043	0.011	0.93	0.013	0.90	3.29	+
C14:0	9	0.447	0.123	0.030	0.94	0.036	0.91	3.42	+
C14:1 cis	10	0.038	0.014	0.008	0.71	0.009	0.63	1.59	-
C16:0	10	1.192	0.400	0.091	0.95	0.106	0.92	3.77	+
C16:1 cis	10	0.065	0.024	0.013	0.73	0.016	0.63	1.51	-
C17:0	8	0.027	0.008	0.003	0.81	0.005	0.67	1.60	-
C18:0	12	0.394	0.137	0.056	0.84	0.064	0.84	2.14	0
C18:1 cis9	9	0.744	0.261	0.061	0.95	0.068	0.95	3.84	+
Total C18:1 trans	13	0.125	0.056	0.025	0.80	0.032	0.73	1.75	-
Total C18:1 cis	9	0.801	0.286	0.063	0.95	0.070	0.95	4.09	+
Total C18:1	10	0.931	0.314	0.060	0.96	0.071	0.96	4.42	+
C18:2 cis9, cis12	10	0.061	0.022	0.011	0.75	0.014	0.65	1.56	-
C18:2 cis 9, Trans 11	10	0.028	0.020	0.010	0.74	0.013	0.69	1.54	-
Total C18:2	9	0.096	0.026	0.014	0.71	0.017	0.63	1.55	-
C18:3 cis9, cis12, cis 15	11	0.020	0.008	0.004	0.69	0.005	0.60	1.56	-
Total of omega 3	11	0.026	0.010	0.006	0.68	0.006	0.64	1.68	-
Total of omega 6	11	0.103	0.028	0.014	0.74	0.018	0.66	1.57	-

Legend
# terms = number of terms (latent variable)
SD = standard deviation of reference values
SEC = standard error of calibration
R^2c = R^2 of calibration
SEP = standard error of prediction
R^2p = R^2 of prediction
RPDp = ratio of SD/SEP. See RPD class

RPD		Class	Application	Symbol
0	2	Very poor	Allows to compare groups of cows, distinguish high or low values	-
2	3	Poor	Screening	0
3	5	Fair	Qualitative screening	+
5	6.5	Good	Quality control	++
6.5	+	Excellent	As precise as reference value	+++

Conclusion

➢Standardisation allows to merge MIR milk spectra from different instruments in the same format.
➢**Common equations were built and can be used by all MIR instruments participating to the standardisation**

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