Extramir spectral proficiency test: comparison of spectral standardisation methods

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The interest of using FT-MIR analysis of milk to predict a large variety of phenotypes (e.g. fine milk quality, health status or environmental impact of cows) is worldwide growing. Such FT-MIR models are tedious and expensive to develop and there is a clear interest in sharing predictive models among organisations of different geographic locations. However, spectral differences between instruments or within instruments across time hinder the sharing and use of common MIR models. To overcome this issue, spectral standardisation methods were developed to harmonise spectral responses of instruments over different networks. The aim of this work was to compare the performances of 4 different spectral standardisation methodologies (Foss, CRAW/EMR, Lactanet and VIT).

Each methodology involved around 10 instruments in the test. Identical sets of 10 milks were distributed by ICAR and analysed by all the spectrometers involved (N=44) to compare their spectral information. A total of 10 FT-MIR models predicting a wide range of phenotypes were applied to all raw and standardised spectra. All these models were developed using spectra standardised with the CRAW/EMR methodology. For each methodology, the spectral and prediction homogeneity across instruments, before and after standardisation, were assessed through the standard deviation of absorbance intensities per wavenumber and the standard deviation of predictions across instruments.

Results highlight the spectral differences between instruments without standardisation and the resulting heterogeneity between predictions of different spectrometers. Overall, the predictions were improved after standardisation for each method in comparison to before standardisation. The 4 standardisation methodologies show different performances in improving the spectral homogeneity between instruments and among spectral regions. Therefore, the performances in harmonising the predictions homogeneity were also different according to methods and models. Finally, the results suggest that differences in spectral standardisation across methodologies may constrain model transferability between networks (i.e. sharing models may require standardising spectra to the same reference to build the model and for predictions). This highlights the need for further research to better understand and potentially overcome these limitations.