

Electronic supplementary material

Development and comparison of regression models for determination of quality parameters in margarine spread samples using NIR spectroscopy

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Table S1: Range and average values of the reference measurements for the four cases.

| Spectral Mode | Range | | Average | |
|---------------|-------------|------------------|---------|------------------|
| | Fat (%) | Dry material (%) | Fat (%) | Dry material (%) |
| Reflectance | 19.3 - 61.3 | 39.7 - 80.7 | 39.2 | 60.5 |
| Transmission | 17.7 - 57.5 | 19.5 - 59.7 | 35.3 | 38.1 |

Table S2: Summary of the performance parameters of the models for the four datasets. Average values were calculated in all cases. RMSEC, RMSECV and RMSEP values are in %. Y means the measured content (dependent variable). RSD is the relative standard deviance in %.

| Spectral mode | Y | R ² | Q ² | RMSEC | RMSECV | LVs | Q ² ext | RMSEP | RSD (RMSEP, %) |
|---------------|--------------|----------------|----------------|--------|--------|-----|--------------------|--------|----------------|
| Reflectance | Fat | 0.9846 | 0.9772 | 1.6214 | 1.9955 | 4 | 0.7735 | 3.1525 | 20.30 |
| | Dry material | 0.9809 | 0.9730 | 1.8140 | 2.2245 | 5 | 0.8824 | 2.4370 | 11.53 |
| Transmission | Fat | 0.9543 | 0.9245 | 2.3378 | 2.8545 | 5 | 0.8507 | 3.3803 | 61.75 |
| | Dry material | 0.9704 | 0.9488 | 1.8676 | 2.2399 | 4 | 0.9199 | 2.8145 | 62.66 |

Figure S1: One example of the evaluated regression models. PLS regression with interval selection (50 splits) was used. The number of PLS components were 5 and random 5-fold CV was applied. Predicted Y values were plotted against the reference Y values. Blue dots are assigned to the calibration and red dots are assigned to the validation set.

