Sample-Specific Prediction Error Measures in Spectroscopy

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Figure S1. Near-infrared spectra obtained on individual wheat kernels. Calibration (blue) and prediction (red) samples.
Figure S2. Singular Value Decomposition of near-infrared spectra obtained on individual wheat kernels. (a) Loadings and (b) scores for the two first principal components (PC). Test set in red, calibration set in blue.
Figure S3. Illustration of the least squares (LS) bias as a function of $y$. 
Figure S4. Underfitted PCR model (four PCs). (a) Measured ($y$) versus predicted ($\hat{y}$) values of protein for calibration samples (blue) and prediction samples (red). Mean squared error of calibration (MSEC) is 0.33 and mean squared error of prediction (MSEP) is 0.33. (b) Estimated bias versus true bias for each specific sample in the prediction dataset. The estimated bias ($E(\hat{y} - y)$) is given by Eq. 11 and the true bias is given by ($\hat{y} - y$). Loess is used for estimating the average tendency. Only samples marked with a red circle, Prediction (included), were included when estimating Loess.