Prediction of crude protein and starch concentrations in ruminal *in situ* studies and ruminal degradation of cereal grains using near-infrared spectroscopy

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**Supplementary Table S1** *Chemical characteristics of grain samples that were used for* in situ *incubations.*

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  |  | n | Mean | Min | Max |
| EE |  |  |  |  |  |
| (% DM) | Barley | 20 | 2.9 | 2.4 | 3.4 |
|  | Durum | 15 | 2.8 | 2.5 | 3.2 |
|  | Maize | 20 | 5.8 | 4.3 | 12.3 |
|  | Peas | 13 | 2.1 | 1.9 | 2.4 |
|  | Rye | 20 | 1.9 | 1.8 | 2.1 |
|  | Triticale | 20 | 1.9 | 1.6 | 2.3 |
|  | Wheat | 20 | 2.2 | 1.9 | 2.5 |
| aNDFom |  |  |  |  |  |
| (% DM) | Barley | 20 | 18.7 | 15.2 | 20.9 |
|  | Durum | 15 | 10.1 | 9.0 | 11.4 |
|  | Maize | 20 | 9.0 | 7.1 | 11.0 |
|  | Peas | 13 | 12.8 | 11.0 | 16.0 |
|  | Rye | 20 | 14.5 | 12.6 | 17.2 |
|  | Triticale | 20 | 13.4 | 10.1 | 16.9 |
|  | Wheat | 20 | 11.8 | 10.1 | 13.5 |
| ADFom |  |  |  |  |  |
| (% DM) | Barley | 20 | 5.6 | 4.5 | 7.1 |
|  | Durum | 15 | 3.5 | 3.0 | 4.0 |
|  | Maize | 20 | 2.8 | 2.1 | 3.2 |
|  | Peas | 13 | 8.4 | 7.3 | 9.8 |
|  | Rye | 20 | 2.9 | 2.4 | 3.4 |
|  | Triticale | 20 | 2.9 | 2.4 | 3.3 |
|  | Wheat | 20 | 3.1 | 2.5 | 3.8 |

EE = Ether extract; aNDFom = Neutral detergent fibre assayed with a heat stable amylase exclusive of residual ash; ADFom = Acid detergent fibre exclusive of residual ash

All analyses performed as described by Rodehutscord *et al.* (2016)

\*LOQ = values lower than the limit of quantification (LOQ for ADL: 0.45% DM)

**Supplementary Table S2** *Parameters describing the performance of NIRS-calibrations for the CP and starch (ST) concentration of grains1) and their bag residues after* in situ *incubation and the effective degradability (ED) of CP and ST of cereal grains at a ruminal passage rate of 5 and 8%/h.*

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Parameter** | **CP** | **ED5CP** | **ED8CP** | **ST** | **ED5ST** | **ED8ST** |
| **Calibration** |  |  |  |  |  |
| Units | % DM | % | % | % DM | % | % |
| SEL | 0.4 | n.a. | n.a. | 1.37 | n.a. | n.a. |
| N | 463 | 85 | 85 | 451 | 85 | 85 |
| Outliers | 7 | 0 | 0 | 9 | 0 | 0 |
| Min | 1.3 | 54.2 | 44.9 | 0.5 | 57.8 | 45.6 |
| Mean | 13.7 | 80.1 | 74.7 | 36.8 | 88.8 | 85.0 |
| Max | 38.2 | 88.8 | 85.6 | 76.5 | 96.1 | 95.7 |
| SD | 5.8 | 9.4 | 11.0 | 23.1 | 11.5 | 14.3 |
| SEC | 0.35 | 1.52 | 1.83 | 1.57 | 1.23 | 1.51 |
| R2C | 1.00 | 0.97 | 0.97 | 1.00 | 0.99 | 0.99 |
| SECV | 0.39 | 2.53 | 3.07 | 1.71 | 2.28 | 2.73 |
| R2CV | 0.99 | 0.92 | 0.91 | 0.99 | 0.96 | 0.96 |
| Number of terms | 15 | 12 | 12 | 14 | 13 | 13 |
| WL range/step | 1250-2450/1 | 1250-2450/1 | 1250-2450/1 | 1250-2450/1 | 730-2450/1 | 1250-2450/1 |
| Pretreatment (s) | 1,8,8 | 1,8,8 | 1,8,8 | 1,8,8 | 1,8,8 | 1,8,8 |
| Regression method | PLS | PLS | PLS | PLS | PLS | PLS |
| **Validation** |  |  |  |  |  |
| N | 150 | 30 | 30 | 150 | 30 | 30 |
| Outliers | 0 | 0 | 0 | 0 | 0 | 0 |
| Min | 4.2 | 54.8 | 45.6 | 0.5 | 58.1 | 47.9 |
| Mean | 14.2 | 80.9 | 74.8 | 34.7 | 89.4 | 85.4 |
| Max | 35.6 | 88.8 | 85.8 | 75.5 | 96.8 | 95.7 |
| SD | 5.8 | 9.4 | 11.0 | 23.8 | 11.3 | 14.4 |
| R2P | 0.99 | 0.96 | 0.95 | 0.99 | 0.96 | 0.97 |
| RMSEP | 0.46 | 1.94 | 2.43 | 2.10 | 2.2.25 | 2.45 |
| SEP(C) | 0.46 | 1.90 | 2.38 | 2.10 | 2.25 | 2.45 |
| Bias | 0.03 | -0.38 | -0.49 | 0.08 | 0.13 | 0.13 |
| Intercept | 0.07 | -0.77 | -0.99 | 0.17 | 0.26 | 0.26 |
| Slope | 1.00 | 1.00 | 1.01 | 1.00 | 1.00 | 1.00 |
| Global Distance Average | 1.2 | 1.0 | 1.5 | 1.1 | 1.4 | 1.5 |
| Nearest Neighbour Distance Average | 0.2 | 0.4 | 0.6 | 0.2 | 0.6 | 0.6 |

SEL = standard error of laboratory; N = number of samples after outliers have been removed; Min, Mean and Max = lowest, mean and highest value of the reference dataset; SD = SD of the reference values; SEC = standard error of calibration; R2C = R2 of the calibration; SECV standard error of cross validation; R2CV = R2 of the cross-validation; WL range/step = wavelength range and steps (nm); Pretreatment (s) = pretreatment of the spectra (deviation,gap, smooth); R2P = R2 of validation; RMSEP =RMSE of the validation; SEP(C) = RMSE of the validation corrected for bias; PLS = partial least square.

1) Cereal grains (barley, durum, maize, rye, triticale, wheat) and peas