

Supplementary Table 2. Different pre-treatments were applied to the raw spectra obtained from the Perkin Elmer Spectrum II FTIR® spectrometer and a PLSR model generated with the transformed spectra and reference values. A calibration set of samples was used to generate each model and was evaluated by an independent validation set of samples. Each model was evaluated based on its calibration R² and RMSE (mg/gDW) values, with those providing the lowest RMSE (mg/gDW) values for the validation set, chosen as the pre-treatment for the final model. The pre-treatments chosen for each variable measured are listed below with the calibration and validation R² and RMSE (mg/gDW) values from that PLSR model.

Cell Wall Component	Calibration R²	Calibration RMSE (mg/gDW)	Validation R²	Validation RMSE (mg/gDW)	Spectral Pre-treatments
Cell wall	0.95	14.59	0.88	16.89	Area Normalisation, Optical Scattering Correction
Total Carbohydrates	0.94	14.99	0.91	17.27	Baseline corrected, Multiple Scattering Correction, 2 nd derivative with 9 smoothing points
Glucan	0.96	9.79	0.96	10.20	Standard Normal Variate, 2 nd derivative with 9 smoothing points
Xylan	0.92	3.99	0.87	6.59	Standard Normal Variate, 2 nd derivative with 9 smoothing points
Arabinan	0.87	1.84	0.64	4.13	Baseline corrected, 2 nd derivative with 1 smoothing points
Galactan	0.87	2.88	0.77	3.78	Standard Normal Variate, 2 nd derivative with 9 smoothing points
Mannan	0.72	1.19	0.41	2.15	2 nd Derivative with 1 smoothing point
Total Lignin	0.93	7.76	0.92	10.86	Area Normalisation, Optical Scattering Correction
ASL	0.96	0.56	0.94	0.84	Baseline, Area Normalized, Second derivative
AIL	0.95	5.57	0.89	12.58	Optical Scattering Correction
Ash	0.97	5.91	0.97	14.00	Baseline, Area Normalized, 1 st derivative