Appendix

Table 1. Calibration and validation statistics for the NREL corn stover feedstock PLS2 model. The statistical summary includes the number of samples in each model, the number of latent variables (LVs) used to develop the model, and the root mean square error of calibration (RMSEC). Also included are the root mean square error of prediction (RMSEP), the square of the correlation coefficient (R²), the slope and intercept for the fully cross-validated prediction models.

Constituent	#Samples	#LVs	RMSEC	RMSEP	R ²	Slope	Intercept
Extractives	107	10	1.37	1.82	0.89	0.87	1.53
Cellulose	107	10	1.05	1.50	0.75	0.75	9.05
Xylan	107	10	0.71	0.87	0.84	0.85	2.98
Lignin	107	10	0.82	1.27	0.56	0.69	4.62

Table 2. Calibration and validation statistics for the NREL mixed herbaceous feedstock PLS2 model. The statistical summary includes the number of samples in each model, the number of latent variables (LVs) used to develop the model, and the root mean square error of calibration (RMSEC). Also included are the root mean square error of prediction (RMSEP), the square of the correlation coefficient (R^2) , the slope and intercept for the cross-validated prediction models.

Constituent	#Samples	#LVs	RMSEC	RMSEP	R ²	Slope	Intercept
Extractives	183	6	2.67	2.83	0.87	0.87	1.82
Cellulose	183	6	2.11	2.26	0.90	0.90	3.25
Glucan	183	6	2.05	2.18	0.89	0.90	3.31
Xylan	183	6	1.35	1.47	0.81	0.81	3.36
Lignin	183	6	1.26	1.35	0.88	0.88	1.86