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Structural study as a support for predictive NIR analysis of multiple pretreated sugarcane bagasse samples for ethanol production

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Biomass conversion yields to ethanol are critically linked to the uncertainties of the structural properties of the pretreated sugarcane bagasse. Thus, a better understanding of lignocellulose composition will allow addressing the factors to make viable an efficient cellulosic fuel economy. Moreover, a rapid analytical method such a near-infrared (NIR) spectroscopy, properly calibrated by chemiometrics, is fundamental for further creation of a consistent library of data. This work presents a quick method for analyzing the chemical composition of sugarcane bagasse, by using coupled with multivariate analysis. NIR sugarcane spectra were collected from pretreated samples obtained from different methods (organosolv, sodium hydroxide and aqueous ammonia). NIR spectra are correlated to compositional data produced using traditional wet chemical analysis. A rapid calibration model is put forth to predict cellulose, hemicellulose and lignin yields of a variety of pretreated sugarcane samples. Both cross-validation and independent validation results showed that the developed broad-based model is promising for future chemical prediction of other pretreated samples. Also, the major structural challenges are represented by cellulose crystallinity and the association of cellulose, lignin and hemicellulose. Complementary, spectroscopic and microscopy techniques can reveal molecular insights of these components. Finally, this paper illustrates an integrated and exhaustive methodology to be used as selection criteria between competitive technological options for processing cellulosic material into ethanol.

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