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Development of near infrared spectroscopy models for the quantitative prediction of the lignocellulosic components of wet *Miscanthus* samples

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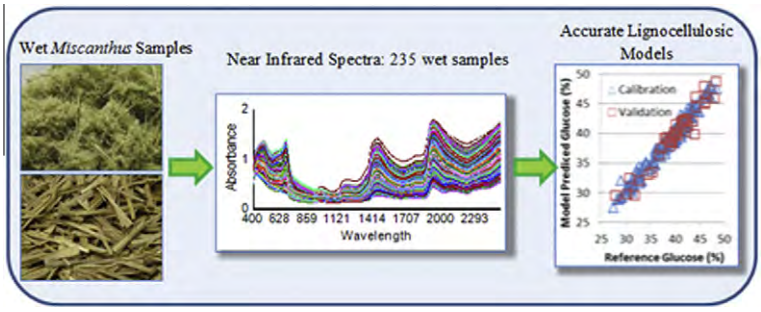
HIGHLIGHTS

- Models developed for lignocellulosic/elemental constituents based on NIR spectra.
- Different models covered wet and dry samples, different particle sizes.
- Models on dry, ground and sieved samples were the most accurate.
- Wet models suitable for quantification: total sugars, glucose, xylose, Klason lignin.
- Other wet models suitable for classification or sample screening.

GRAPHICAL ABSTRACT



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ABSTRACT

Miscanthus samples were scanned over the visible and near infrared wavelengths at several stages of processing (wet-chopped, air-dried, dried and ground, and dried and sieved). Models were developed to predict lignocellulosic and elemental constituents based on these spectra. The dry and sieved scans gave the most accurate models; however the wet-chopped models for glucose, xylose, and Klason lignin provided excellent accuracies with root mean square error of predictions of 1.27%, 0.54%, and 0.93%, respectively. These models can be suitable for most applications. The wet models for arabinose, Klason lignin, acid soluble lignin, ash, extractives, rhamnose, acid insoluble residue, and nitrogen tended to have lower R^2 values (0.80+) for the validation sets and the wet models for galactose, mannose, and acid insoluble ash were less accurate, only having value for rough sample screening. This research shows the potential for online analysis at biorefineries for the major lignocellulosic constituents of interest.

1. Introduction

Miscanthus is a perennial C_4 rhizomatous grass that has been grown as an energy crop. Numerous varieties have been grown experimentally (Clifton-Brown et al., 2001) but fewer commercially. In Ireland *Miscanthus* × *giganteus* is the only crop established commercially, although in countries with colder winters *Miscanthus* × *sinensis* has been grown. In recent years there has been interest in utilising *Miscanthus* as a feedstock (Haverty et al., 2012; Melligan et al., 2012) in lignocellulosic biorefining technologies (Hayes, 2008) for the production of biofuels and chemicals. The yields in these processes will depend on the composition of the feedstock (Hayes and Hayes, 2009) which will change according to the productivity of the plant and its time of harvest (Lewandowski et al., 2003). However, the wet-chemical analytical protocols, as outlined in Section 2, are costly and time-consuming. Hence, accurate and robust rapid methods of analysis could be of value, particularly if integrated online in a biorefinery.

The combination of near infrared spectroscopy (NIRS) (750–2500 nm) and chemometric techniques (e.g., partial least squares regression (Wold et al., 2001)) has allowed for numerous models for the rapid analysis of forage and grains to be developed (Shenk and Westerhaus, 1994). There have also been studies on developing NIR models for the lignocellulosic and elemental

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