Determination of Silica in Wheat Leaves with ATR-FTIR-Chemometrics

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Although plant scientists have noted the beneficial effects of silicon for over 150 years, only during the last decades its role in high productivity agriculture systems has been thoroughly studied. The presence of silicon in plants contributes to the response of stress-relief mechanisms for environmental events such as drought and pathogen attack. Because of the importance of crops such as wheat, barley, rice, and other grasses that accumulate Si, the understanding of the relationship between this element and plant science is the focus of numerous scientific efforts. However, quantification of this element is a difficult and costly task; destructive wet chemistry methods followed by spectrophotometry are commonly used.

In this work, we developed a nondestructive and cheap method for silicon determination using infrared spectroscopy and chemometrics. Dried wheat leaves grown in a greenhouse were analyzed by means of attenuated total reflection infrared spectroscopy (ATR-FTIR) and inductively coupled plasma-optical emission spectroscopy elemental analysis (ICP-OES).

A series of models based on multivariate ordinary least squares regression using varying sets of wave numbers selected by a genetic algorithm, was built using baseline corrected ATR-FTIR spectra from wheat leaves samples. Models built with these sets showed a powerful correlation with the silicon content determined by elemental analysis. The performance in prediction of each model was assessed using repeated k-fold cross validation, showing a maximum error of prediction (RMSEP) of 0.1% wt. with minimum model complexity of 4 selected variables. However a strong dependence on the matrix was noted when compared with other plant tissues.

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