Determination of Silicon in Wheat Leaves with ATR-FTIR and Chemometrics

Felipe Beltran - Yohana Cabrera - Andres Cabrera

The beneficial effects of silicon for plants have been noticed for more than a century, but only during the last two decades has its role in high productivity agriculture systems thoroughly studied. The presence of silicon in plants contributes to stress-relief mechanisms for environmental events such as drought and pathogen attacks. Because of the importance of crops such as wheat, barley, rice, and other grasses that accumulate Si, understanding the relationship between this element and plant science is the focus of numerous scientific efforts. Si quantification is a difficult and costly task, and destructive wet chemistry methods are commonly used. With the recent development of chemometric tools, analysis of silicon in complex matrices has been proved feasible for certain matrixes.

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

Using varying sets of wave numbers selected by a genetic algorithm, a series of models based on multivariate ordinary least squares regression was built using baseline-corrected ATR-FTIR spectra from wheat leaves samples. Models built with these sets showed a strong 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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