Brachiaria plantaginea (Link) Hitchc. as a Potential (New) Source of Shikimic Acid. Quantification by NIR and PLS Regression

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Abstract

Shikimic acid is a natural compound, precursor of the antiviral *Oseltamivir* used against influenza A. It is a scarce and expensive chemical, obtained mainly from seeds of shrubs natives in China and Japan. In this study we propose a fast and clean procedure for the quantification of shikimic acid in *B. plantaginea*, an alternative source of shikimic acid, using NIR spectroscopy combined with PLS regression.

Introduction

This study shows the results of shikimic acid accumulation in *Brachiaria plantaginea*, abundant grassy in Brazil and other countries in Africa and America, after glyphosate spraying at three different doses. Forty four samples of *B. plantaginea* were analyzed and shikimic acid was quantified by high performance liquid chromatography (HPLC). Although HPLC is quantitative and precise, it can also be time-consuming and costly, requiring large quantities of expensive and toxic organic solvents.[1]

The main objectives of this study were investigate the glyphosate dose and exposure period of the *B. plantaginea* to the herbicide that would result in the greatest accumulation of shikimic acid; then, propose a fast and clean procedure for the quantification of shikimic acid in samples of *B. plantaginea* using NIR spectroscopy combined with PLS regression.

Results and Discussion

The herbicide glyphosate was sprayed at reduced doses of 36.0, 3.6 and 0.36 g acid equivalent (a.e.) of glyphosate ha^{-1}. The determination of shikimic acid in *B. plantaginea* leaves was performed at 3, 6, 9 and 12 days after treatments. The results show a higher accumulation of shikimic acid after 6 days of glyphosate application at the concentration of 36.0 g acid equivalent of glyphosate ha^{-1}, which are consistent with the literature.[2]

Spectra of 44 samples were obtained using diffuse reflectance mode in the range of 4000 to 10000 cm^{-1} with 4 cm^{-1} resolution. Different mathematical pretreatments were applied to the spectra, and the data were mean-centered. The calibration model (7 factors) exhibited coefficient of determination, R^2 = 0.9930 (*SEC* = 84.05). For external validation, R^2 = 0.9317 and *SEP* = 154.91. For external validation, the mean prediction error was 10% and the range error ratio (*RER*) was 9.42, indicating that the model is qualified for screening calibration.

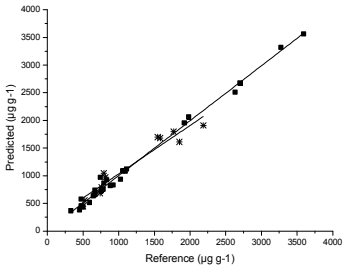

Figure 1. Plot of reference *vs*. predicted values for (■) calibration and (⁎) external validation of shikimic acid in *B. plantaginea* samples models (7 factors).

Conclusions

The reasonable agreement between reference *vs*. predicted values for calibration and external validation sets indicates that the final model can be used for an approximate prediction of new samples. The difficulty in getting a better model can be explained in part by the wide range of shikimic acid concentrations (333.9 to 3592.45 µg g^{-1}). Despite of the difficulty to establish a PLS model for this data set, the results were satisfactory, demonstrating that NIR spectroscopy associated to PLS regression is a possible alternative to quantify shikimic acid in *B. plantaginea*.

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