The use of infrared spectroscopy for prediction of nitrogen and nitrate composition in plant materials

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Applications of Fourier Transform infrared (FTIR) technology for the rapid and cheap prediction of soil analytes are well known. For agronomical applications, the extension of the technique for the assessment of total nitrogen and nitrate composition in plant material is highly attractive, especially if the same infrared spectrometer can be used for both. The main objective of this study is to report on the usefulness of infrared spectroscopy for the prediction of nitrogen and nitrate composition in a range of plant materials associated with agronomy. A total of 357 plant samples (including barley, pears, potato, tomato, wheat and a range of other horticultural plant species) were analysed for nitrate and nitrogen content. Dried and ground plant were scanned with a benchtop Fourier Transform infrared (FTIR) instrument (Thermo Nicolet iS-50 (Thermo Inc., USA) in diffuse reflectance mode. Predictive partial least square regressions (PLSR) were developed by leave-one-out cross-validation using the spectral and analytical information. Models were based on the full spectral range (8000-450 cm-1), the near-infrared (NIR 8000-4000 cm-1) and mid-infrared (MIR 4000-450 cm-1) were compared by assessing their coefficients of determination (R2) and root mean square errors of cross-validation (RMSECV). Our results show that nitrogen was predicted well with both the MIR (R2 = 0.96 and RMSECV = 0.034 %) and NIR (R2 = 0.96 and RMSECV = 0.032 %) with MIR requiring less factors (12 vs 15), and nitrate was predicted with high accuracy in the MIR (R2 = 0.98 and RMSECV = 156 mg/kg) with slightly less accuracy in the NIR (R2 = 0.95 and RMSECV = 210 mg/kg). The nitrate data was dominated by high concentrations associated with potato petioles and therefore accuracy for other crop types still needs to be explored.