Direct rapid analysis of trace bioavailable soil macronutrients by chemometrics-assisted energy dispersive X-ray fluorescence and scattering spectrometry

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Abstract

Precision agriculture depends on the knowledge and management of soil quality (SQ), which calls for affordable, simple and rapid but accurate analysis of bioavailable soil nutrients. Conventional SQ analysis methods are tedious and expensive. We demonstrate the utility of a new chemometrics-assisted energy dispersive X-ray fluorescence and scattering (EDXRFS) spectroscopy method we have developed for direct rapid analysis of trace 'bioavailable' macronutrients (i.e. C, N, Na, Mg, P) in soils. The method exploits, in addition to X-ray fluorescence, the scatter peaks detected from soil pellets to develop a model for SQ analysis. Spectra were acquired from soil samples held in a Teflon holder analyzed using 109Cd isotope source EDXRF spectrometer for 200 s. Chemometric techniques namely principal component analysis (PCA), partial least squares (PLS) and artificial neural networks (ANNs) were utilized for pattern recognition based on fluorescence and Compton scatter peaks regions, and to develop multivariate quantitative calibration models based on Compton scatter peak respectively. SQ analyses were realized with high CMD ($R2 > 0.9$) and low SEP (0.01% for N and Na, 0.05% for C, 0.08% for Mg and 1.98 g g^{-1} for P). Comparison of predicted macronutrients with reference standards using a one-way ANOVA test showed no statistical difference at 95% confidence level. To the best of the authors' knowledge, this is the first time that an XRF method has demonstrated utility in trace analysis of macronutrients in soil or related matrices.