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Usefulness of NIR spectroscopy for the estimation of the mineral composition and texture of soils and heavy metal uptake

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The accumulation of heavy metals in soils from different sources (atmospheric deposition, agricultural practices, urban-industrial activities, etc.) is of a great environmental concern. In this sense, there is a consensus in the literature that the total heavy metals in soil are not a suitable tool for risk assessment regarding heavy metal mobility and bioavailability. Several approaches have been proposed to estimate this bioavailability but controversy exists to define an universal method. The bioavailability is influenced, apart from other properties like pH, organic matter, etc., by the mineral fraction and texture of a soil. However, the determination of these parameters, especially the mineral composition, is laborious, expensive, and time consuming. Thus, the objectives of this work are the estimation of the texture and mineral components of contrasting soils and the heavy metal uptake (Cu, Zn, Pb, Ni, Cr, Cd) by barley after sewage sludge application using NIR spectroscopy.

A set of 70 contrasting soils from different parts of Spain were used for the analysis of the texture and mineral composition. The mineralogical characterization of soil samples was carried out by X-ray diffraction (XRD) using whole soil random powder, oriented clay on ceramic plates, and clay random powder. Chung method was used for semi-quantitative interpretation of X-ray diffraction patterns of soils, obtaining the percentage of Calcite (Ca), Quartz (Q), Albite (Ab), Potassium Feldspar (FK), phyllosilicates (PS). For the prediction of heavy metal uptake, the 70 soils were divided in two separate sets of 36 (experiment 1) and 34 (experiment 2) soils. The methodology for both experiments, separated in time, was the same. The soils were amended with the same dose of sewage sludge (15.71 g dry weight kg-1) and placed in pots. In these pots, a bioassay with barley, under greenhouse conditions, was carried out. Eight weeks after sowing, the plants were harvested. Roots were dried in an oven at 65ºC for 2 days, and total heavy metals were determined.

The soil samples (air-dried and ground to pass through 2-mm sieve) were placed in glass Petri-dishes, and scanned on reflectance mode from 12000 to 3800 cm-1. For these measurements, a Fourier-Transform near infrared (FT-NIR) spectrophotometer (MPA, Bruker Optik GmbH, Germany) was used. Partial least squares (PLS) regressions were performed to relate the spectral information with the studied parameters.

For the mineral parameters and texture, and according to the RPD value, the following models were obtained: excellent for Ca (R2=90.33; RPD=3.24) and Ab (R2=86.03; RPD=2.70), very good (where quantitative predictions are possible) for silt (R2=77.61; RPD=2.13), sand (R2=75.46; RPD=2.03), Q (R2=75.72; RPD=2.04) and FK (R2=78.97; RPD=2.20), and fair models which may be used for assessment and correlation for clay (R2=68.19; RPD=1.78) and PS (R2=67.63; RPD=1.77).

For the case of the estimation of the heavy metal uptake, and using the results obtained in the experiment 1, very good models were obtained for Pb (R2=80.75; RPD=2.31), fair, where only high and low values are distinguishable, Ni (R2=50.13; RPD=1.43) and Cd (R2=57.65; RPD=1.56), and poor for Cu (R2=21.94; RPD=1.15), Zn (R2=1.03; RPD=1.02) and Cr (R2=46.01; RPD=1.38). The models developed with the results obtained in the experiment 2 were classified as follows: excellent for Zn (R2=87.62; RPD=2.89) and Ni (R2=85.67; RPD=2.68), very good for Pb (R2=75.08; RPD=2.04) and Cd (R2=77.37; RPD=2.13), good for Cu (R2=72.54; RPD=1.94), and fair for Cr (R2=54.9; RPD=1.51). Although satisfactory results were found for Cu and Zn in the experiment 2 (surprisingly, after the bad results of the experiment 1), they seemed not to be useful, since they were influenced by just one high value, very different to the rest. However, this was not the case of the rest of studied metals, which seemed to have similar patterns in both experiments, with logical differences due to the different ranges, soils, etc.

The results indicate that NIR spectroscopy can be a very useful tool to estimate some mineral components and texture of soils but further analyses including a higher number of samples should be performed. For the case of heavy metal uptake, and according to the low number of samples and the observed differences between experiments, it is just possible to conclude that, although it seems that NIR spectroscopy could estimate the phytoavailability of some metals, greater efforts must be done.

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