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Prediction of Ba, Co and Ni for tropical soils using diffuse reflectance spectroscopy and X-ray fluorescence spectroscopy

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Environmental impact assessments may be assisted by spatial characterization of potentially toxic elements (PTEs). Diffuse reflectance spectroscopy (DRS) and X-ray fluorescence spectroscopy (XRF) are rapid, non-destructive, low-cost, prediction tools for a simultaneous characterization of different soil attributes. Although low concentrations of PTEs might preclude the observation of spectral features, their contents can be predicted using spectroscopy by exploring the existing relationship between the PTEs and soil attributes with spectral features. This study aimed to evaluate, in three geomorphic surfaces of Oxisols, the capacity for predicting PTEs (Ba, Co, and Ni) and their spatial variability by means of diffuse reflectance spectroscopy (DRS) and X-ray fluorescence spectroscopy (XRF). For that, soil samples were collected from three geomorphic surfaces and analyzed for chemical, physical, and mineralogical properties, and then analyzed in DRS (visible + near infrared - VIS+NIR and medium infrared - MIR) and XRF equipment. PTE prediction models were calibrated using partial least squares regression (PLSR). PTE spatial distribution maps were built using the values calculated by the calibrated models that reached the best accuracy using geostatistics. PTE prediction models were satisfactorily calibrated using MIR DRS for Ba, and Co (residual prediction deviation - RPD > 3.0), Vis DRS for Ni (RPD > 2.0) and FRX for all the studied PTEs (RPD > 1.8). DRS- and XRF-predicted values allowed the characterization and the understanding of spatial variability of the studied PTEs.