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Feasibility of diffuse reflectance infrared Fourier spectroscopy (DRIFTS) to quantify iron-cyanide (Fe-CN) complexes in soil

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Contaminated sites create a significant risk to human health, by poisoning drinking water, soil, air and as a consequence food. Continuous release of persistent iron-cyanide (Fe-CN) complexes from various industrial sources poses a high hazard to the environment and indicates the necessity to analyze considerable amount of samples. At the present time quantitative determination of Fe-CN concentration in soil usually requires a time consuming two step process: digestion of the sample (e.g., micro distillation system) and its analytical detection performed, e.g., by automated spectrophotometrical flow injection analysis (FIA). In order to determine the feasibility of diffuse reflectance infrared Fourier spectroscopy (DRIFTS) to quantify the Fe-CN complexes in soil matrix, 42 soil samples were collected (8 to 12.520 mg kg-1CN) indicating single symmetrical CN band in the range 2092 - 2084 cm-1. Partial least squares (PLS) calibration-validation model revealed IR response to CNtot exceeding 1268 mg kg-1 (limit of detection, LOD). Subsequently, leave-one-out cross-validation (LOO-CV) was performed on soil samples containing low CNtot (<900 mg kg-1), which improved the sensitivity of the model by reducing the LOD to 154 mg kg-1. Finally, the LOO-CV conducted on the samples with CNtot >900 mg kg-1 resulted in LOD equal to 3494 mg kg-1. Our results indicate that spectroscopic data in combination with PLS statistics can efficiently be used to predict Fe-CN concentrations in soil. We conclude that the protocol applied in this study can strongly reduce the time and costs essential for the spatial and vertical screening of the site affected by complexed Fe-CN.