



Use of near infrared reflectance spectroscopy (NIRS) for determining soil content in chlorddecone (organochlorine pesticide)

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Chlorddecone is a toxic organochlorine insecticide that was used in banana plantations until 1993 in the French West Indies. Now previously contaminated soils have become new sources of contamination for natural water and cultivated roots and tubers, and represent an important concern of public health, at last in the French West Indies. The conventional method for analyzing chlorddecone in soils involves extraction with two solvents and quantification by gas chromatography-mass spectroscopy (GC-MS), which has a low detection limit but is expensive, and the whole process takes several hours. This does not easily allow analyzing large amounts of samples such as those required for characterizing soil contamination and its variations on vast areas. Near infrared reflectance spectroscopy (NIRS) has been reported to allow accurate prediction of diverse soil properties. The present study aimed at assessing the potential of NIRS for characterizing soil contamination by chlorddecone over a set of 236 samples collected at 0-30 and 30-60 cm depths in Andosols (109 samples), Nitisols (72 samples) and Ferralsols (55 samples) from Martinique. Over the set, chlorddecone content ranged from 0 to 20 mg kg⁻¹.

Using partial least square regression, chlorddecone content determined through GC-MS could be correctly predicted by NIRS ($Q^2 = 0.73$, $R^2_{val} = 0.82$, $RPD = 2.2$ for the total set), especially for samples with chlorddecone content < 12 mg kg⁻¹, or when the sample set was rather homogeneous ($Q^2 = 0.78$, $R^2_{val} = 0.91$, $RPD = 3.0$ for the Andosols). Conventional measures and NIRS predictions were poorly correlated for chlorddecone content > 12 mg kg⁻¹ (which is huge), suggesting under-prediction by NIRS. Nevertheless, when the set was divided into three or four classes of chlorddecone content (< 5 , 5-10 and > 10 , or < 5 , 5-10, 10-15 and > 15 mg kg⁻¹, respectively), contamination class was correctly predicted for ca. 80% samples.

In addition, looking at B-coefficients (i.e. regression coefficients in the equation that expresses chlorddecone content as a function of absorbance at every wavelength) indicated that wavelengths around 1830-1840 nm contributed heavily to the prediction of chlorddecone content by NIRS. The 1860 nm region has been attributed to the absorption due to the sixth overtone of C-Cl bond stretching, which could be linked to the fact that the molecule of chlorddecone includes ten C-Cl bonds (its formulae is $C_{10}Cl_{10}O$). This strongly suggests that chlorddecone content was directly predicted by NIRS, though it was very low.

Thus NIRS could be considered a time- and cost-effective method for characterizing soil contamination by chlorddecone in the soils from Martinique.