



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

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Chlordecone 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 least in the French West Indies. The conventional method for analyzing chlordecone 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 chlordecone 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, chlordecone content ranged from 0 to 20 mg kg<sup>-1</sup>.

Using partial least square regression, chlordecone content determined through GC-MS could be correctly predicted by NIRS ( $Q^2 = 0.73$ ,  $R_{val}^2 = 0.82$ , RPD = 2.2 for the total set), especially for samples with chlordecone content < 12 mg kg<sup>-1</sup>, or when the sample set was rather homogeneous ( $Q^2 = 0.78$ ,  $R_{val}^2 = 0.91$ , RPD = 3.0 for the Andosols). Conventional measures and NIRS predictions were poorly correlated for chlordecone content > 12 mg kg<sup>-1</sup> (which is huge), suggesting under-prediction by NIRS. Nevertheless, when the set was divided into three or four classes of chlordecone content (< 5, 5-10 and > 10, or < 5, 5-10, 10-15 and > 15 mg kg<sup>-1</sup>, 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 chlordecone content as a function of absorbance at every wavelength) indicated that wavelengths around 1830-1840 nm contributed heavily to the prediction of chlordecone 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 chlordecone includes ten C-Cl bonds (its formulae is C<sub>10</sub>Cl<sub>10</sub>O). This strongly suggests that chlordecone 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 chlordecone in the soils from Martinique.