E92 The Classification of Forensic Soil Evidences by Application of Thermally Assisted Hydrolysis and Methylation With Pyrolysis-Gas Chromatography/Mass Spectrometry (THM-Py-GC/MS) and Multivariate Analysis

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The goal of this presentation is to discuss the following findings of this study: (1) GC/MS could be applied by *in situ* methylation of low volatile Soil Organic Matters (SOM) contained in a small amount of soil without complicated preparation; (2) the variation in the amount of soil was minimized by data normalization; (3) the chemotaxonomic marker compounds could be determined; and, (4) the data could be statistically interpreted confidently for soil classification. In this study, THM-Py-GC/MS produced many compounds due to the high complexity of SOM.

This presentation will impact the forensic science community by illustrating how SOM profiling can be used as a complement to mineralogical techniques in statistically classifying soil evidences and in finding chemotaxonomic marker compounds in forensic soil classification.

The forensic classification of soil samples was performed by THM of SOM using Py-GC/MS).[1] In this work, 33 THM derivatives were detected as SOM contained in <3mg soil.[2] Soil was *in situ* thermally hydrolyzed and methylated with Tetramethylammonium Hydroxide (TMAH) in pyro-foil. The specific ions of the mass spectra were selected to separate and minimize the interference between SOM peaks. SOM data were normalized with the sum of peak areas to correct the amounts of SOM contained in the soil, and the chemometric approach based on Principal Component Analysis (PCA), Hierarchical Cluster Analysis (HCA), and Linear Discriminant Analysis (LDA) was employed to evaluate and compare the soil classification.[3] The first seven Principal Components (PCs) accounted for 94.8% of the total cumulate variance and these PCs were statistically determined by multiple comparisons (Tamhane's T2 and Dunnett's T3) for the post hoc test (p-value <0.05) and were used to construct the LDA model. It was determined that multiple comparisons (Tamhane's T2 and Dunnett's T3) were a statistically good criterion for deciding on the number of PCs for the LDA model. It was also concluded that the discrimination model correctly classified 40 soil samples into six clusters with high accuracy. Furthermore, the 11 marker compounds were investigated according to the loadings of PCs and the normalized data. It was found that six clusters are differentiated by the presence of lignin, fatty acids, and urea.

This method can provide some advantages: (1) GC/MS could be applied by *in situ* methylation of low volatile SOM contained in a small amount of soil without complicated preparation; (2) the variation in the amount of soil was minimized by data normalization; (3) the chemotaxonomic marker compounds could be determined; and, (4) the data could be statistically interpreted confidently for soil classification.

In this study, THM-Py-GC/MS produced many compounds due to the high complexity of SOM. To differentiate soils, PCA, HCA, MC, and LDA were performed to extract the information necessary to characterize soil groups. These results demonstrated that lignin, fatty acid, and urea can be used as potentially useful compounds to characterize soil samples for forensic purposes. These results represent a preliminary investigation of trace organic matter present in soil. It is believed that SOM profiling can be used as a complement to mineralogical techniques in statistically classifying soil evidence and in finding chemotaxonomic marker compounds in forensic soil classification.

Reference(s):

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