



A145 Discrimination of Ignitable Liquids from Matrix Interferences Using Chemometric Procedures

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After attending this presentation, attendees will understand the objective method for the discrimination of ignitable liquid residues (ILRs) from burned matrix interferences using chemometric procedures. Pearson product moment correlation (PPMC) coefficients and principal components analysis (PCA) are used to demonstrate the discrimination of an ignitable liquid from matrix interferences as well as the association of the extracted liquid to its neat counterpart.

This presentation will impact the forensic community by providing a more objective method for analyzing ignitable liquid residues (ILRs) in forensic arson investigations, thereby minimizing the incidence of misidentification or misclassification of ILRs.

In arson investigations, ignitable liquids and ILR extracts are routinely analyzed by gas chromatography-mass spectrometry (GC-MS), and the resulting chromatograms are visually examined to identify the class of ignitable liquid present. However, identification of the ILR is complicated by numerous factors including weathering and evaporation of the ignitable liquid during the fire, the presence of inherent hydrocarbons in the matrix, and the presence of pyrolysis and degradation products formed during the burning process. Such interferences further complicate visual assessment of chromatograms and comparisons with reference collections of neat liquids. Because of these issues, an objective method is necessary to distinguish ignitable liquids from burned matrices and thereby minimize the risk of false positive identifications.

The purpose of this research was to develop an objective method using PPMC coefficients and PCA not only to distinguish an ILR from a burned matrix, but also to associate the ILR with its neat counterpart. The first step in this research was to explore GC-MS temperature programs to determine the fastest program that did not compromise the discrimination afforded. This temperature program was then used for all subsequent analyses by GC-MS. A reference collection of neat ignitable liquids was then compiled, consisting of ignitable liquids from six different ASTM classes: gasoline, petroleum distillates, isoparaffinic, naphthalenic paraffinic, n-alkane, and aromatic products. The ignitable liquids were extracted with activated carbon strips and the resulting extracts were analyzed by GC-MS to generate total ion chromatograms (TICs) and extracted ion profiles (EIPs) of characteristic compound classes.

The potential of PPMC coefficients and PCA for the association and discrimination of ignitable liquids from the same and different classes based on the TICs and EIPs was then investigated. PPMC coefficients were calculated to evaluate the pairwise association of ignitable liquids from the same and differing classes while PCA was used to identify natural clusters in the neat ignitable liquid data set. In the PCA scores plot, ignitable liquids from the same class were clustered closely while different classes were clustered distinctly. Loadings plots were used to determine the chemical components of the ignitable liquids that contributed the most variance to determine if other extracted ion profiles may offer increased discrimination.

A reference collection of four unburned and burned household matrices (carpet, fabric furniture upholstery, magazine, and cotton clothing) was then compiled to identify inherent hydrocarbons, pyrolysis products, and degradation products. The matrices were extracted using activated carbon strips and the resulting extracts were analyzed by GC-MS.

To examine the effects of these matrix interferences on the identification of an ignitable liquid in simulated fire debris, a set of six ignitable liquids was spiked onto each of the four matrices and burned. These spiked and burned matrices were extracted and the extracts were analyzed by GC-MS using the same procedures as previously mentioned. The chromatograms of the spiked and burned matrices were compared to those of the corresponding neat ignitable liquid and burned matrices. PPMC coefficients were calculated to assess the association and discrimination afforded between pairs of chromatograms based on the TIC and each EIP. PCA was then applied to investigate the possibility of associating the burned ILR to the corresponding neat liquid and discriminating from matrix interferences. In the burning process, the majority of the volatile components are lost, which was reflected in the TIC and some EIPs, such as the aromatic profile. Other EIPs, including the alkane EIP, were unaffected by the burning process, and hence were more useful in associating to the neat ignitable liquid, while discriminating from matrix interferences.

Ignitable Liquids, Chemometrics, Arson