A32 A Study of Complex Mixtures From Fire Debris by Summed Ion Spectra

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After attending this presentation, attendees will comprehend the complexity of fire debris analysis and appreciate the use of summed ion spectra from GC-MS analysis to quickly compare reference liquids to fire debris samples.

This presentation will impact the forensic science community by elucidating information about the complex mixtures of ignitable liquids and substrate materials found in fire debris.

In fire debris analysis, a complex mixture is extracted from fire debris, which may contain an ignitable liquid residue and pyrolysis products from burned substrates at the fire scene. Typically, these complex mixtures are analyzed by gas chromatography - mass spectrometry producing a 3D data file [m/z, time (scan), and intensity axes]. Total ion and extracted ion chromatograms are generated from the time and intensity data and are comprised of a series of peaks where each peak is a constituent in the complex mixture. Pattern recognition of a total ion chromatogram is the basis for classifying an ignitable liquid residue according to the ASTM E1618 standard method. A complementary method of summing the intensity of each m/z across the chromatographic time range produces a summed ion spectrum. The summed ion spectra allows for rapid automated searching against a library of reference spectra and a measurement of similarity between the spectra. An ignitable liquid residue spectrum can be compared to libraries of ignitable liquid and burned substrate reference spectra.

Summed ion spectra were created from existing GC-MS data files obtained in the Ignitable Liquid Reference Collection (ILRC) database. Summed ion spectra of pyrolysis products from substrates were obtained from the GC-MS data of burned substrate materials. Similarity comparisons between normalized summed ion spectra were performed by custom software written in-house. The automated search produces a list of library entries and their similarity with the sample spectrum in rank order from most similar to least similar. When searching against both ignitable liquid and substrate libraries, the search produces a list of the most similar combination of ignitable liquid reference and burned substrate reference spectra with the percentage of their relative contributions to the sample spectrum. A comparison of summed ion spectra similarities was performed by cluster analysis based on the Euclidean distance between the similarity measurements. This study compared: (1) ignitable liquids within the same ASTM classification; (2) weathered ignitable liquid spectra to their corresponding un-weathered liquid spectra; (3) burned substrate spectra; and, (4) burned substrate spectra to ignitable liquid spectra. Automated searches of summed ion spectra against ignitable liquid and burned substrate reference libraries were conducted on fire debris samples.

The results indicate ignitable liquids can be further grouped by various classifiers within given ASTM classifications. Cluster analysis demonstrates weathered ignitable liquids were more similar to their corresponding un-weathered ignitable liquid than to other ignitable liquids. Gasolines with the same amount of weathering were more similar to one another than their corresponding un-weathered gasoline. Cluster analysis demonstrates the majority of products from burned substrate materials are not similar to one another. The majority of ignitable liquids are not similar to the products of burned substrate materials tested. Results from automated searching of a fire debris sample spectrum against ignitable liquid and burned substrate reference libraries contained numerous high similarity matches with ignitable liquids of the same ASTM classification, except for liquids in the light carbon range.

Software developed at UCF can rapidly perform the comparisons between complex mixtures found in fire debris based on their summed ion spectra. Large libraries of spectra can be compared to elucidate information about these complex mixtures. The software can be applied to compare fire debris sample spectra to libraries of ignitable liquid and burned substrate reference libraries for ASTM classification and/or identification of the ignitable liquid residue.

Fire Debris, Complex Mixtures, Summed Ion Spectra

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