B75 Identification of Potential Target Compounds in Fire Debris

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After attending this presentation, attendees will better understand the chemical composition of fire debris from the identification of compounds within ignitable liquid residues and pyrolysis/combustion products from substrate materials.

This presentation will impact the forensic science community by providing information that can be utilized in determining the presence and classification of ignitable liquid residues by identifying potential target compounds.

Fire debris analysis is conducted to determine whether an ignitable liquid residue is present in the fire debris collected from the scene. One challenge to making this determination is the presence of decomposition products from the pyrolysis and combustion of substrate materials at the scene. Some of these decomposition products are extracted along with ignitable liquid residues to form a complex mixture of compounds from both. In 1991, Keto and Wineman developed a method for the analysis and identification of selected target compounds.[1] They identified target compounds from the American Society for Testing and Materials (ASTM) E 1618 classifications of gasoline, medium petroleum distillates, and heavy petroleum distillates.[2] They obtained semi-quantitative Gas Chromatography/Mass Spectrometry (GC/MS) peak areas for these target compounds to construct Target Compound Chromatograms (TCCs). The study determined that TCC for gasoline, medium petroleum distillates, and heavy petroleum distillates were different from those of plywood and carpet with padding. TCCs enable the analyst to visualize low concentrations of ignitable liquid residues in high concentrations of decomposition products.

The study being presented is based on the identification of potential target compounds in all ASTM E 1618 classes and in decomposition products from substrate materials.[2] The data consists of 660 neat ignitable liquids and 106 burned substrate materials from the Ignitable Liquids Reference Collection (ILRC) and the Substrate Databases.[3,4] A library containing retention time and mass spectra of 255 standards has been developed for identification of major peaks within ignitable liquids and substrates in the databases.[3,4] Identification of these compounds within the 766 samples is performed by Target Factor Analysis (TFA), which calculates a correlation between the spectrum of the sample and the 255 test spectra. Logistic regression is performed to convert the correlations to probabilities. When a probability is larger than a specific threshold, that compound is identified as being present in the sample. A maximum likelihood frequency of occurrence in ignitable liquids and substrates is tabulated for each of the 255 compounds. Compounds with a high frequency of occurrence in ignitable liquids and a low frequency of occurrence in decomposition products from burned substrate materials are potential target compounds. This concept can also be applied for each ASTM E1618 class of ignitable liquid.[2]

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Reference(s):

1. Keto R.O., Wineman P.L. Detection of Petroleum-Based Accelerants in Fire Debris by Target Compound Gas Chromatography/Mass Spectrometry. *Analytical Chemistry.* 1991; 63(18).\
2. ASTM, *E1618-11 Standard Test Method for Ignitable Liquid Residues in Extracts from Fire Debris Samples by Gas Chromatography-Mass Spectrometry*. 2014, ASTM International: West Conshohocken, PA.
3. The Ignitable Liquids Reference Collection Database can be found at the universal resource locator. Available from: http://ilrc.ucf.edu.
4. The Substrate Database can be found at the universal resource locator. Available from http://ilrc.ucf.edu/substrate/.

Fire Debris, Target Compounds, Ignitable Liquids