A29 Automated Searching of Ignitable Liquids Database by Summed Ion Spectra

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After attending this presentation, attendees will understand this method efficiently utilizes the information contained within a gas chromatographic-mass spectral data file. The gas chromatographic - mass spectral data files contain data used to create a summed ion spectrum which retains sufficiently high information content that it can be used for automated database searches of complex mixtures such as ignitable liquids.

This presentation will impact the forensic community by providing a complementary method to current fire debris analysis methods which follow ASTM E1618 standard method. The method of summing the intensity of each ion across the entire chromatographic range allows for rapid automated searching against a database of ignitable liquid spectra and a measurement of similarity between the ignitable liquid summed ion spectra. Furthermore, background "matrix" effects can sometimes be accounted for to aid in recognition and identification of ignitable liquid residues.

In fire debris analysis, the chromatographic patterns of total ion and extracted ion chromatograms are used to classify an ignitable liquid according to the ASTM E1618 standard method. A complementary method of summing the intensity of each ion across the entire chromatographic range allows for rapid automated searching against a database of ignitable liquid spectra and a measurement of similarity between the ignitable liquid summed ion spectra. Furthermore, background "matrix" effects can sometimes be accounted for to aid in recognition and identification of ignitable liquid residues.

Summed ion spectra were created from existing GC-MS data files obtained in the Ignitable Liquid Reference Collection (ILRC) database. Similarity comparisons between the normalized summed ion spectrum of an ignitable liquid sample and a database of ignitable liquid summed ion spectra were performed by custom software written in-house. The automated search produces a list of database entries and their similarity with the ignitable liquid sample in rank order from most similar to least similar. A similarity measurement between the summed ion spectra of 62 ignitable liquids was calculated. Cluster analysis based on the Euclidean distance between the similarity measurements was performed to determine if ignitable liquids within the same ASTM E1618 classification, as assigned by the Ignitable Liquids Reference Collection Committee, would cluster together. The ability of the database search method to correctly identify an ignitable liquid, its ASTM class and sub- class was evaluated by receiver operating characteristic (ROC) analysis. Since none of the time related data is retained within the summed ion spectrum, it was proposed that summed ion spectra of the same ignitable liquid analyzed by different analytical methods and instruments could be identified, provided that both analytical techniques capture data on ignitable liquid components over the same volatility range. Ignitable liquids of each ASTM classification were analyzed several times utilizing various analytical methods on several different instruments. The comparison of these summed ion spectra for ignitable liquid identification, ASTM classification and sub-classification was evaluated by ROC analysis.

The results indicate the summed ion spectra of complex mixtures contain enough information to make comparisons between ignitable liquids by calculating a simple similarity metric. The cluster analysis demonstrates ignitable liquids that predominately contain alkanes are similar to one another. It also indicates ignitable liquids containing alkanes are more similar to ignitable liquids with isoalkanes than ignitable liquids containing aromatics. Duplicate analyses of the ignitable liquids have an extremely high probability of being correctly identified with the correct class and sub-class assignments having a lower probability of being correct. Analyses of the same ignitable liquids with various analytical and instrumental methods had slightly lower probabilities of correct associations than those analyzed by the same analytical method and instrument. Identification of specific product types within a broader ASTM classification and sub-classification is possible because each product contains a mixture of components in unique ratios. Each component has a unique EI mass spectrum and the resulting sum of spectra is similarly unique.

The software developed at UCF can rapidly perform the comparisons between an ignitable liquid sample summed ion spectra and a database of ignitable liquid summed ion spectra, typically searching a database of 450 entries in a fraction of a second. The database search results can assist in the determination of the ASTM classification and sub- classification of an ignitable liquid sample. The method is also applicable in the discrimination of questioned and known samples of complex mixtures. The summed ion spectral comparison method with the in-house software is being evaluated by the State of Florida Bureau of Forensic Fire and Explosives Analysis. The software has been applied to assist investigators in one missing person case and has been used to analyze and discriminate between commercial explosives.

The summed ion spectral comparison with associated software provides a complementary method to the ASTM E1618 standard method typically utilized in fire debris analysis, and may find utility in many additional physical evidence comparisons.

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