B153 The Identification of Representative Compounds in Ignitable Liquids and Substrates: Classification of Fire Debris Using a Naïve Bayes Approach

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After attending this presentation, attendees will better understand the classification of fire debris as positive or negative for the presence of ignitable liquid residue using a Naïve Bayes approach.

This presentation will impact the forensic science community by utilizing a method for the identification of representative compounds in fire debris and the determination of the presence or absence of ignitable liquid residue in fire debris using likelihood ratios. The purpose of the presentation is to propose a classification system for fire debris.

In this study, 700 burned and 100 unburned substrates and 646 neat ignitable liquids were used. The burned substrate samples were prepared using Modified Destructive Distillation Method (MDDM), Direct Heat (DH), and Indirect Heat (IH) methods. Identification of the compounds in the chromatograms of the substrate and ignitable liquid samples were analyzed by Automated Mass Spectrometry Deconvolution and Identification System (AMDIS) software, using a library containing 282 compounds, including the retention times, retention indices, and mass spectra of each compound.[1]

Logistic regression and Receiver Operating Characteristic (ROC) analysis were applied to evaluate the probability of the presence of the library compounds in substrates and ignitable liquids. For these calculations, the delRT (1/[1+| Δr.t.|]) parameter was introduced. This parameter uses the absolute value of the retention time difference (|Δr.t.|) between the compound in the library and the sample. The data used to generate the logistic regression model was comprised of multiple compounds from each of 42 ignitable liquids taken from the Ignitable Liquid Reference Collection (ILRC) database.[2] Liquids were selected from all American Society for Testing and Materials (ASTM) E1618-14 classes.[3] ROC analysis was used to determine the best logistic regression model. Compounds having a probability ≥0.75 were designated as being present in the sample.

Based on their estimated presence or absence, the frequencies of occurrence of the compounds in substrates and ignitable liquids were calculated as the number of occurrences divided by the total number of ignitable liquid or substrate samples. For example, methanol was identified 13 times in 624 substrate samples. Therefore, the frequency of occurrence of methanol in substrates is 2.1×10^{-2}. Some compounds were found to have a zero frequency of occurrence in substrates or ignitable liquids. For instance, acrolein was found to have a zero frequency of occurrence in ignitable liquids. Failure to observe a compound in ignitable liquids or substrates is the result of the statistical sample and not a true estimate of the frequency of occurrence in the population. The Good-Turing smoothing technique was used to estimate the probabilities of occurrence for the compounds that were not seen in the substrates and ignitable liquids.

The frequency of occurrences obtained for the 282 library compounds in substrates and ignitable liquids were used to calculate likelihood ratios for the presence of ignitable liquid in a fire debris sample using a Naïve Bayes approach. The likelihood ratio is calculated by Naïve Bayes as the ratio of the product of the probabilities of occurrence in ignitable liquids (numerator) and substrate (denominator) for each of the 282 compounds found in a fire debris sample. Results will be presented for the cross validation of the method and testing on fire debris data.

This research was supported by the National Institute of Justice, Office of Justice Programs. The findings and opinions expressed in this work are those of the authors and do not reflect those of the United States Department of Justice.

Reference(s):

1. The new Automated Mass Spectrometry Deconvolution and Identification System (AMDIS): http://chemdata.nist.gov/mass-spc/amdis/.
2. Ignitable Liquids Reference Collection Database: http://ilrc.ucf.edu/.
3. Standard Test Method for Ignitable Liquids Residues in Extracts from Fire Debris Samples by Gas-Chromatography-Mass Spectrometry. ASTM International, 2014.

Fire Debris, Logistic Regression, Naive Bayes

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