B143 The Development of an Internet-Deployed Statistical Application for the Analysis of Compounds in Fire Debris Samples

Michelle Corbally, MS, National Center for Forensic Science, Orlando, FL 32828; Jessica Chappell, PhD, Alexandria, VA 22303; Mary R. Williams, MS, National Center for Forensic Science, Orlando, FL 32816-2367; Michael E. Sigman, PhD, University of Central Florida, Orlando, FL 32816*

Learning Overview: After attending this presentation, attendees will understand how to interpret data using an internet-deployed statistical application developed to analyze fire debris samples for compounds found in substrates and ignitable liquids.

Impact on the Forensic Science Community: This presentation will impact the forensic science community by demonstrating the importance of using user-friendly statistical applications for the analysis of fire debris samples. This application provides a streamlined method for determining the presence, in fire debris, of up to 295 commonly identified compounds found in ignitable liquids and substrates. Compounds were identified by Target Factor Analysis (TFA) and required to meet or exceed a decision threshold based on a Fisher z-score identified by decision theory.

The application first converts the retention times of chromatograms into retention indices using a hydrocarbon ladder to allow for interlaboratory sample analysis. Peaks were detected in the Total Ion Chromatogram (TIC) and Extracted Ion Profiles (EIPs) based on second derivative maxima with intensities that exceeded ±2.5 standard deviations from the mean. For a compound to be identified as corresponding to a chromatographic peak, two criteria are required to be met. The first criterion is that the compound being identified is within a ±11.157 retention index range of the library compound that is being identified within the chromatogram. The second requirement is that the Fisher transform of the Pearson product moment correlation coefficient between the library Mass Spectral (MS) target factor and the vector resulting from projecting the target factor into the PC space meets or exceeds the optimized Fisher z-score threshold. The acceptable retention index range was based on commonly observed peak widths in the Ignitable Liquids Reference Collection (ILRC) database and Substrate databases. The optimal Fisher score was determined from receiver operating characteristic analysis of a set of standard-verified compounds in ignitable liquid and substrate samples to determine the optimal decision threshold.

The National Center for Forensic Science (NCFS) ILRC and Substrate database records were also analyzed using the statistical method implemented in the application to determine the frequency at which the 295 compounds were found in an ignitable liquids and substrates. Approximately 1,050 ignitable liquids at different stages of weathering and 553 substrates burned using a Modified Destructive Distillation Method (MDDM) were analyzed. The retention times were converted to retention index using the slope and y-intercept of the retention times of the n-alkanes in American Society for Testing and Materials (ASTM) E1618 Test Mix Standard Reference Material (SRM) 2285.

The tool is deployable on the internet as a Shiny application and is synergistic with current fire debris analysis methods based on ASTM E1618. The target factor analysis used in the application developed from this research aspires to contribute an objective means for fire debris analysts to identify ignitable liquid and substrate compounds in fire debris samples.

This project was supported by Award Number 2019-DU-BX-0016 awarded by the National Institute of Justice, Office of Justice Programs, United States. Department of Justice. The opinions, findings, and conclusions or recommendations expressed in this presentation are those of the authors and do not necessarily reflect those of the Department of Justice.

Fire Debris, Target Factor Analysis, Chemometrics