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Development of an expert system for classifying ignitable liquid residues in fire debris by ASTM E1618

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Abstract

The ASTM E1618 Method establishes criteria for the fire debris analyst to classify ignitable liquid residues into one of eight different classes based on visual inspection of extracted ion chromatograms from GCMS data. Some cases require identification of specific compounds based on mass spectra. We have developed an expert system which predicts which class based on the same extracted ion chromatograms. The data set used for this expert system is the complete Ignitable Liquid Reference Collection (ILRC) maintained by National Center of Forensic Science (Univ. of Central Florida) and Technical Working Group for Fire and Explosives (TWGFEX) of 548 commercial products representing all classes under E1618 which either may be used as an accelerant in commission of arson or be incidental liquids found in fire debris. Like mass spectral library search programs, a similarity index is provided as a measure of confidence in the classification. Also like any search or matching algorithm, the analyst should confirm the match by his/her own inspection of the data. Classification from preliminary tests give correct assignment greater than 95% (lowest for oxygenate and miscellaneous classes) and the correct classification was listed in the top three picks for IRLC samples. E1618 standard recommends identification of specific compounds based on mass spectral matches for these classes especially when only a few compounds are present. The expert system works with only extracted ion data rather than full mass spectral data. These classes as well as samples resulting in a low match are flagged for analyst attention and verification of assignment. Aside from inclusion of an internal standard (3-phenyl toluene) in the carbon disulfide solvent used in the activated charcoal method (E1412), no special columns or temperature programs are required. The extracted ion chromatograms are exported from GCMS software as comma separated variables (CSV) and imported into the expert system thus is vendor independent. The retention time and area counts of the internal standard are added as the first line in the data file. The internal standard is used to determine relative retention times of individual components and only semi-quantitative measure of the concentration of individual compounds. Data from an E1618 standard mix is used to determine the “high”, “medium” or “low” subclasses of each E1618 class. The expert system and data processing software are written in the free open source statistical software language R (http://www.r-project.org/). The expert system was tested using actual fire debris samples where the ignitable liquid known was independent of the training data set or as diluted liquids simulating evidence collected from a container. Effect of substrate on classification will be presented.

Biography

J. Graham Rankin received his BS in Biology from Southern Methodist University, a Ph.D. in Oceanography from Texas A&M. Following a 14 year career with the R&D arm of Shell Oil in Houston, he returned to academia earning a Ph.D. in Analytical Chemistry from the University of Houston. Upon graduation he joined the Chemistry Department at Marshall University in 1993. He was asked to be on the faculty advisory committee for the Forensic Science Program at its inception and began giving occasional lectures there with the first class in 1995. In 2000, he joined the program full time and developed the forensic chemistry emphasis in that program. He is a Fellow in the American Academy of Forensic Science, and a member of the Mid-Atlantic Academy of Forensic Scientists, the American Chemical Society, the E30 Committee on Forensic Science of the ASTM international, and the Technical Working Group for Fire and Explosives (TWGFEX). He is also an associate editor for the *Journal of ASTM International*. He is certified by the American Board of Criminalists as a fire debris analyst and drug analysis.

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