B80 Use of Principal Components Analysis in the Individualization of Smokeless Powders

J. Graham Rankin, PhD* and Joy Cottle, BS, Forensic Science Program, Marshall University, 1401 Forensic Science Drive, Huntington, WV 25701; Cynthia Wallace, BS, Bureau of Alcohol, Tobacco, Firearms & Explosives, National Research Laboratory, 6000 Ammendale Road, Ammendale, MD 20705

After attending this presentation, attendees will understand the applicability of principal components analysis to forensic samples

This presentation will demonstrate the increased awareness of multivariate statistical analysis of large data sets in establishing similarity/dissimilarity between evidence and exemplars.

Traditionally, some smokeless powders can be identified to manufacturer and brand based on physical measurement of particle size and shape. Chromatographic analyses by GCMS, HPLC or MEKC have been shown to further distinguish samples. While some products are quite similar from lot to lot, others vary widely, complicating both brand identification and individualization to the lot level. Recent legal challenges to forensic evidence have stressed the need for statistical metrics for similarity and/or dissimilarity for comparison of evidence and exemplars.

To meet this need, a series of over 200 smokeless powders from the ATF smokeless powder collection have been analyzed for their extractable organic constituents by HPLC-DAD and GCMS. Use of multivariate statistical techniques, such as principal component analysis (PCA), demonstrates that among double base powders, the combination of nitroglycerin, 2,4 dinitrotoluene (2,4DNT), and dibutyl phthalate concentrations can be used to distinguish the various powders tested. Among single base powders, the 2,4DNT, methyl and ethyl centralite concentrations distinguish those powders. Greater than 95% of the variance among the powders can be explained using these few analytes. Cluster diagrams are useful in showing the degree of similarity or dissimilarity among the powders. Examples distinguishing among different lots of the same brands will be given.

Smokeless Powder Analysis, Principal Components Analysis, Explosives