A30 Statistical Analysis of Visible Absorption Spectra and Mass Spectra Obtained From Dyed Acrylic Fibers

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After attending this presentation, attendees will learn more about the applications of statistical analysis to the comparison of fiber dye spectra.

This presentation will impact the forensic science community by presenting an objective method for the comparison of absorption profiles in which spectral similarity is assessed at a known significance level.

Among various techniques, fiber examiners presently utilize microspectrophotometry to obtain the absorption spectra of known and questioned samples. Comparison of the questioned and known spectra is relatively straightforward when absorption profiles are visually distinct, but the task becomes more challenging when dyes exhibit highly similar absorption profiles. A recent report by the National Academy of Sciences indicated the need for the forensic science community to "minimize the risk of results being dependent on subjective judgments." Hypothesis testing provides an objective method of comparing absorption profiles and assessing their similarity at a known significance level.

The objective of this study is to examine the levels of Type I and Type II error for fiber discrimination based on hypothesis testing using parametric and nonparametric analysis of visible absorption spectra and ESI mass spectra. Samples of blue acrylic yarn from different sources were used in this study, two pairs of which came from the same manufacturer but had different color names. Samples were chosen to represent yarns that, in bulk, were considered visually indistinguishable by color. No identifying information about the yarn dyes was known. *In situ* dye absorption profiles were obtained using microspectrophotometry. Dye extracted from the fibers was also used to collect absorption profiles and mass spectra.

Microspectrophotometry measurements in the visible spectral region were collected using spectrometers interfaced to a polarized light microscope (PLM). Several fibers were taken from each yarn source, with each fiber cut into segments and multiple measurements taken along the length of each segment. For analysis of the extracted dyes, fiber segments were heated in a solvent system of pyridine-acetic acid-water (20:5:75, v/v). The extracts were evaporated and resolvated with methanol for absorption spectral and direct infusion electrospray ionization mass spectrometry analysis. Appropriate blanks were prepared and analyzed under the same conditions.

Normalized absorption spectra of the dyes in the fibers were analyzed using a parametric test, which assumes normal distribution of the test statistic, and a non-parametric permutation test, which is not bound by this restriction and guarantees the specified significance level. In hypothesis testing, rejection of the null hypothesis when it is true is considered a Type I error, while failing to reject the null hypothesis when it is false indicates a Type II error. Type I and Type II error will be discussed for segments taken from the same fiber, for different fibers taken from the same source, and for fibers taken from different sources. The sensitivity of this statistical approach will also be discussed in terms of how instrumental parameters and sampling method may affect the error rates. Results from the parametric and non-parametric tests will also be compared. In addition, selected ion intensities from the mass spectra of the extracted dyes were normalized and analyzed using principal components analysis (PCA). PCA scores were compared using cluster analysis based on the Euclidean distance. Hypothesis testing methods will also be investigated for the analysis of this data.

This research was conducted at the National Center for Forensic Science, a State of Florida Type II research center.

Statistics, Fiber Dyes, Microspectrophotometry

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