



### A22 Analysis of Synthetic Polymers Using MALDI-TOF

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The goal of this presentation is to demonstrate the need for objective identification of synthetic polymers in the trace evidence realm of forensic science and to propose the analysis of the fragmentation patterns of these polymers obtained from MALDI-TOF mass spectra to be used for fiber identification.

This presentation will impact the forensic science community by providing an objective method for trace evidence analysis and identification of synthetic fibers.

Synthetic fibers, or polymers, are created through addition or condensation reactions that combine monomers. Each manufacturer may introduce various chemical additives, which affect the chemical and physical properties of the material. Such additive categories include: flame retardance; dyes, pigments; UV absorbers and antioxidants; plasticizers; surfactants; and lubricants. Each manufacturer is at liberty to distinguish their product with various additive combinations. However, these additive combinations are not able to be used for identification purposes with the current analysis techniques for synthetic fibers. Current methods of analysis include: visual comparison and microscopy, which are both subjective identification techniques, and Fourier transform infrared spectroscopy (FTIR), which identifies the polymer into a general type. Fiber evidence collected from a crime scene can provide valuable information in the investigation of the crime. However, it is often not a critical piece of evidence due to the lack of objective identification of fiber source. Trace fiber evidence can come from many different sources that often appear identical through the above mentioned analyses. This makes it nearly impossible to determine a source of origin. A synthetic fiber database classified by polymer type and manufacturer additives could objectify fiber analysis by narrowing and confirming the fiber's source of origin. This creates a need for an analytical technique that can ultimately identify the fiber type and manufacturer source. Matrix-assisted laser desorption ionization (MALDI) is a mass spectrometry analytical technique that utilizes a laser beam to ionize the analyte, in this case the fiber. The absorbing matrix is mixed with the sample, allowing the analyte and the matrix to co-crystallize on the target plate. The matrix uses the energy provided from the laser to desorb itself from the target, pulling analyte particles with it into the gas phase as ions. In ion form, the analyte particles are then carried to the mass spectrometer detector, the time-of-flight (TOF) mass spectrometer. The TOF works by accelerating the ions toward the drift region where all ions have the same kinetic energy but different masses, thereby separating based solely on particle size. The goal of this research is to provide an objective identification procedure through the use of MALDI-TOF analysis that can distinguish various synthetic polymers based on the individual manufacturers' additives. MALDI-TOF was used to determine the polymer additive composition for comparison of similar polymer types. Optimized MALDI parameters were obtained for nylon, olefin, and polypropylene to produce mass spectra with high resolution and complete peak separation. This was obtained by spotting the target with a salt solution comprised of trifluoroacetic, sodium salt in tetrahydrofuran (THF) followed by a matrix solution, comprised of  $\alpha$ -cyano-4-hydroxy-cinnamic acid (CHCA) in THF. The optimized parameters were then used to obtain two sets of mass spectra for four differently manufactured nylon fibers using the matrices, CHCA and trans-2-[3-(4-tert-Butylphenyl)-2-methyl-2-propenylidene] malononitrile (DCTB). These same fibers were also analyzed using FTIR as a comparison. The FTIR results confirmed the fiber identity as nylon, but could not distinguish any differences between the different manufactured nylon fibers. The MALDI-TOF mass spectra were analyzed to distinguish between matrix peaks, polymer peaks, and chemical additive peaks. When comparing spectra obtained for nylon against the spectra for the matrices CHCA and DCTB, there were similar peaks present that were not attributed to the matrix. Further analysis is required to detect spectral differences due to additive composition of differently manufactured polymers. However, when compared to FTIR analysis, this method provides a possible successful objective method for synthetic fiber analysis and identification.

**Synthetic Polymer, Matrix-Assisted Laser Desorption Ionization, Manufacturer Additives of Synthetic Polymers**