Supplementary Material (ESI) for The Analyst

Electronic Supplementary Information for Qualitative and Quantitative Analysis of Explosives and Drugs from Fabrics by Ambient Mass Spectrometry by Nari Talaty, Christopher C. Mulligan, Dina R. Justes, Ayanna U. Jackson, Robert J. Noll, and R. Graham Cooks.

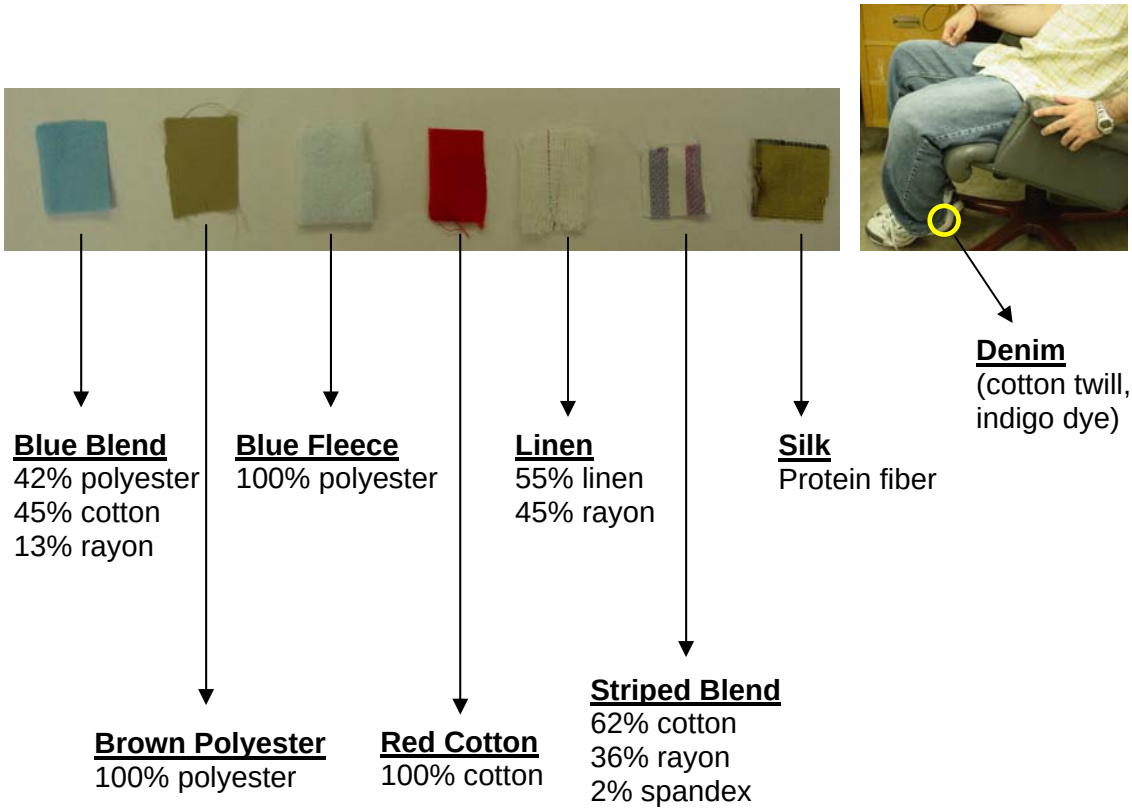

Figure S-1. Fabric samples studied and their compositions. Denim was sampled directly from the cuff of an unwashed pair of blue jeans.

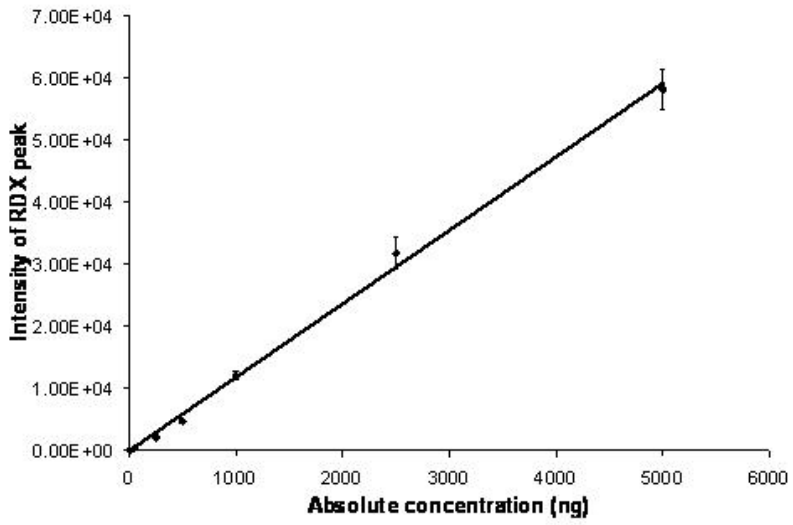

Figure S-2. High-throughput calibration curve for RDX using automated 1D stage. RSDs are 6-10% in working range with decent linearity.

Using an automated 1-D stage, DESI mass spectra could quickly be obtained from each sample (~3 min.) for calibration purposes. Figure S-2 in shows a relatively large linear dynamic range for the analysis of RDX on cotton (at concentrations of 5, 50, 250, 500, 1000, 2500, and 5000 ng/cm^2. The movement of the stage is controlled by software and allows positioning the DESI spray on a single spot for a desired amount of time. The procedure used was similar to surface rastering, but with predetermined dwell time on the center of each fabric sample, and there is little to no carry-over by scanning in order of increasing RDX concentration. Relative standard deviation (RSD) values for this analysis were determine to be 6-10%,

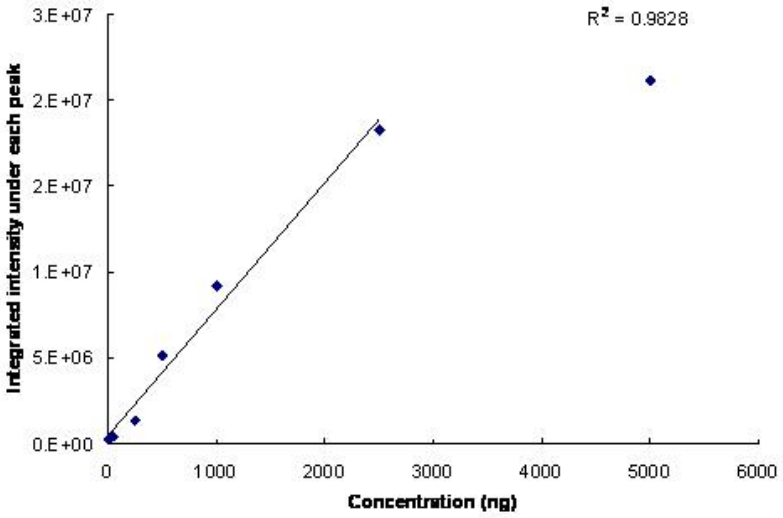

Figure S-3. Quantitation of cocaine on fabric using the total integrated intensity for analyte signal obtained in the chronogram and plotted vs. concentration.

Quantitation of cocaine showed the best linear dynamic range using a ratio of cocaine intensity to that of an internal standard (See Figure 8). Exclusively using the signal intensity for protonated cocaine for quantitation also yields good linearity (R^2= 0.9894), but leads to a decreased linear dynamic range (Figure S-3).