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Forensics Applications of Secondary Ion Mass Spectrometry

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Our government is always in need of precise tools that can rapidly and accurately characterize explosive compositions. At the Environmental Molecular Sciences Laboratory (EMSL) at PNNL, we have state-of-the-art facilities containing a unique suite of analytical tools: some of which are not located anywhere else in the world. Developing these facilities and tools for national security interests will help our government both prevent, and respond to terrorist acts in a timely manner.

Here we describe recent efforts at PNNL to develop a classification method for characterization of explosives using some of these tools, with composition C-4 plastic explosive as a model system. This classification process involves the collection of a unique combination of molecular and elemental signatures with multiple methods. These methods; including Secondary Ion Mass Spectrometry (SIMS), electro-spray ionization fourier transform ion-cyclotron resonance mass spectrometry (ESI-FT-ICR), nano Desorption Electrospray Ionization (nano-DESI) and high throughput Energy Dispersive X-Ray analysis (EDX), have been used to characterize 17 composition C-4 explosive samples obtained from varying locations around the country. The results indicate that each method individually is able to differentiate between *certain* C-4 samples, but not *all*. However, when combined using an advanced Bayesian statistical analysis approach, the data from these methods provides a robust signature combination for each of the C-4 samples analysed.

Mass spectrometric imaging methods, such as SIMS and DESI provide a particularly powerful means for identification and characterization of explosives[1,2].[1,2] A demonstration is given in Figure 1, which shows a large area SIMS map acquired from a human fingerprint, created after handling an ammonium nitrate salt. Ammonium nitrate, and other salts are of particular interest because they are commonly used in explosive devices. These salts can be very difficult to detect using more conventional approaches. However, SIMS can readily detect the signatures of these and other non-volatile materials used in explosives. The green regions in the image represent mass spectral features from fingerprint oils, while the red and yellow regions in the image are signatures characteristic of the ammonium nitrate salt. The blue regions in the image are attributed to the Si substrate.

Figure 2 shows the mass spectral data acquired from RDX crystals in two separate human fingerprints after handling two different types of C-4 plastic explosive; a commercial brand, and a military brand C-4. Both mass spectra contain peaks characteristic of RDX, lipids from the fingerprint oils, and a surfactant contaminant. However, only one of the samples contains the explosive HMX. This is consistent with known compositions of the material.

Overall, these results indicate that imaging mass spectrometry can be a potentially powerful forensic method; one that can be used simultaneously as a biometrics tool with unparalleled specificity.

References:
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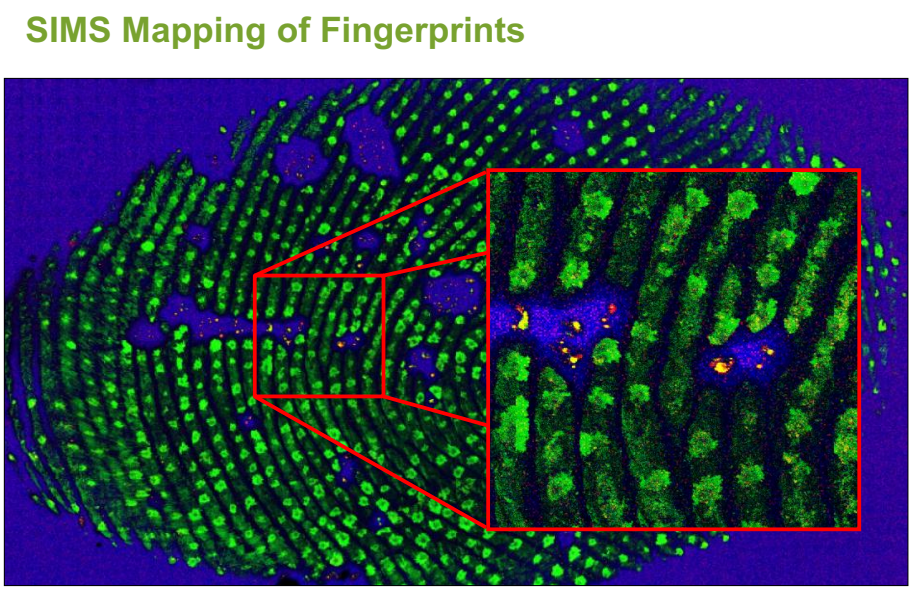

Figure 1. Imaging of chemical constituents in a human fingerprint on Si after handling ammonium nitrate, a salt potentially used in explosives. Green regions: fingerprint oils, yellow/red regions: ammonium nitrate signatures, and blue regions: substrate signal.

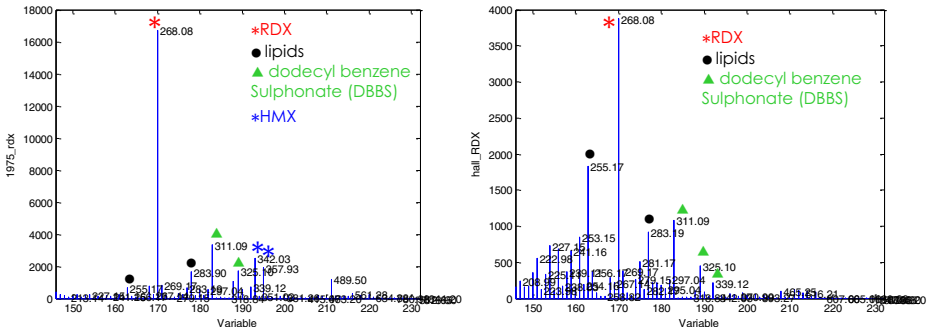

Figure 2. Negative secondary ion mass spectra obtained from RDX particles in a human fingerprint after handling two different types of composition C-4 explosive: Left panel – military C-4 / Right panel – commercial C-4

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