Sticking It to Collection and Analysis: Utilizing Pressure-Sensitive Adhesive Paper Combined with Portable Mass Spectrometry for Detection of Threats

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Abstract

Robust sample collection and identification of dangerous amounts of compounds outside of a laboratory environment is a challenge facing police, first responders, and field forward military units. Additionally, trace amounts of some of these compounds pose severe health hazards. While ionization techniques have been developed to detect several of these compounds, a simple, robust, field friendly method for sample collection is lacking. One way to approach this challenge is to use a modified substrate that can capture, hold, and be directly analyzed.

Herein, we demonstrate the usefulness of pressure-sensitive adhesive (PSA) substrates, i.e. yellow sticky notes, to directly capture trace analytes from a variety of surfaces leading to identification on a portable MS instrument. Regular PSA paper was previously shown to be optimal for sample analysis. Cocaine, fentanyl, methamphetamine, XLR-11, TNT, RDX, and HMX were identified by paper spray ionization (PS-MS) using the PSA substrate on typical laboratory instruments. The LODs for these compounds was < 50pg. In order to demonstrate the effectiveness of the PSA substrate to increase surface collection, five different surfaces were spotted with the three drugs and sampled. Unmodified paper and paper coated with PSA were dabbed onto the spots and analyzed after a labeled internal standard was added. In all cases, the PSA substrate gave significantly higher signal to background ratios with p values < 0.05. The LODs for the five compounds collected from the tested surfaces was in the low nanogram range with robustness to common interferents.

The direct sampling/analysis methods were next transitioned to a portable mass spec instrument. PS-MS and atmospheric pressure chemical ionization (APCI) were both utilized for analysis for transitioning to on-site/field forward threat identification. Both of these ionization methods required minimal to no sample preparation prior to analysis. All the examined threat agents were identified by on the portable instrument. Sample analysis took less than 1 minute for PS-MS and ~10 seconds for APCI. A MATLab/Python script was developed for quantitation. The LODs for analytes on the substrates was <50ng using the Bayspec. After analysis, sufficient analyte remained on the PSA substrate to allow for confirmation using Gold Standard confirmatory identification benchtop instrumentation out to 4 weeks later.

Threat identification was presented to the user using either mass spectrums or a Red Light/Green Light signal. These different end points allowed the user to quickly to alerted of a hazard/threat in the field environment and to save the spectrum for further evaluation.

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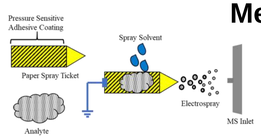
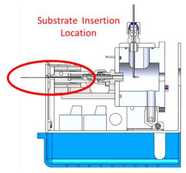
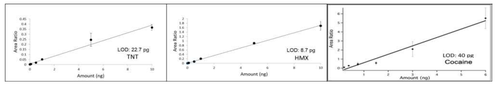
Methods





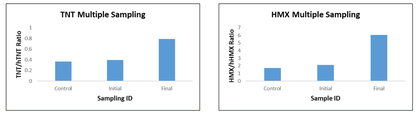
HRMS



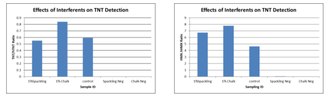
Compounds	S:B ratio									
	Asphalt		Cloth		Concrete		Glass		Metal	
	PSA	*Paper*	*PSA*	*Paper*	*PSA*	*Paper*	*PSA*	*Paper*	*PSA*	*Paper*
Cocaine	1872	115	13194	6539	1060	21.8	2839	185	3062	305
Fentanyl	3988	23.9	87958	172	82	2.9	580	13.4	682	17
XLR-11	158	20.9	14900	1655	249	2.8	8135	0.4	6095	28.1

Compounds	Asphalt	Cloth	Concrete	Glass	Metal
	LOD (ng)	*LOD (ng)*	*LOD (ng)*	*LOD (ng)*	*LOD (ng)*
Cocaine	2.58	1.51	3.89	0.55	0.29
Fentanyl	3.15	5.88	6	4.53	2.16
XLR-11	2.4	2.59	4.39	4.48	1.21
TNT	Not Tested	31.8	Not Tested	5.3	15.5
HMX	Not Tested	43.1	Not Tested	5	8.9

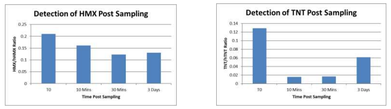
Multiple Sample Events



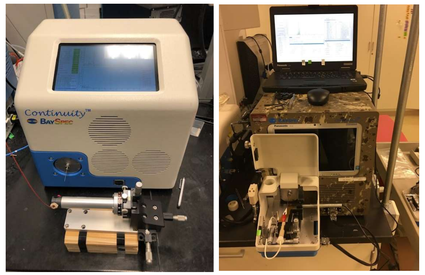
Interferents

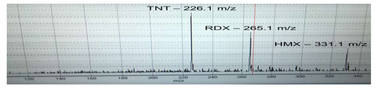


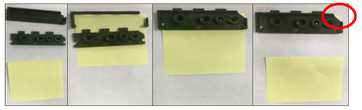
Sample Stability

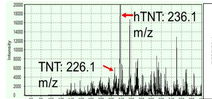


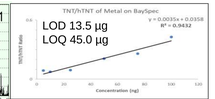
Mini-MS

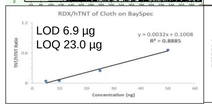


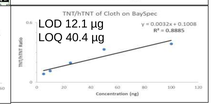






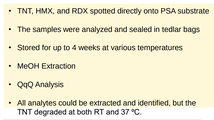


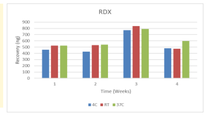


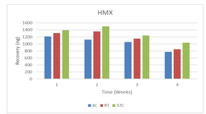


Reanalysis

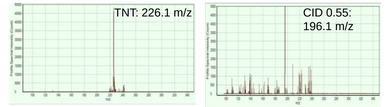
- TNT, HMX, and RDX spotted directly onto PSA substrate
- The samples were analyzed and sealed in tedlar bags
- Stored for up to 4 weeks at various temperatures
- MeOH Extraction
- QqQ Analysis
- All analytes could be extracted and identified, but the TNT degraded at both RT and 37 °C.





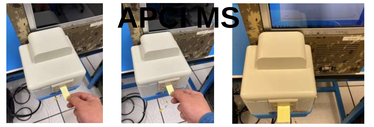


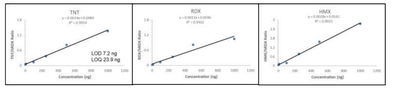
MS/MS Analysis



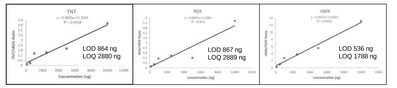
Green Light / Red Light

APCI MS





APCI Surface Sampling

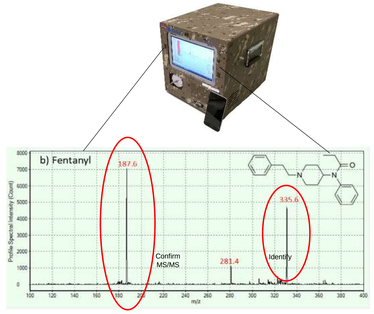


Conclusions

- Sticky notes can capture and hold threat analytes
- Robust Sampling
- Mini-MS MS/MS analysis
- Surface LODs < 1µg
- Extraction and reanalysis of Substrates
- APCI analysis to eliminate Spray Solvent
- Green Light / Red Light Endpoint

Next Steps

- Stick Notes vs TSA Swabs
- Field Testing
- Library Builds
- User Feed Back
- Team with Raman



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