TECH NOTE 1.0

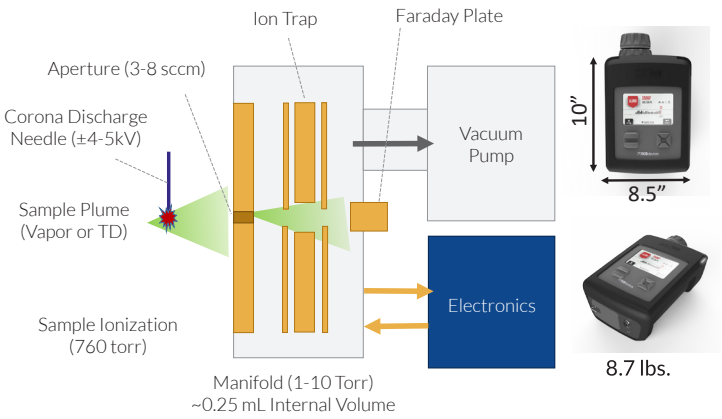
Next-Generation Handheld High-Pressure Mass Spectrometry (HPMS) with an APCI Dual-Polarity Source for Threat Detection

Overview

Many military, law enforcement, and first responder missions can benefit from enhanced in situ, chemical analysis. Chemical analysis performed in these mission areas are often constrained by requirements including high confidence in the result, low limits of detection, and, in some cases, high sample throughput. Transitioning large-scale laboratory instruments that readily meet these requirements into field portable tools has been an active area of development now for several years. Historically, mass spectrometers with ambient ionization sources readily meet the performance specifications that field applications require, however the need to operate at high vacuum imposes severe penalties on power (battery size), start-up time, cost, and simplicity of operation and maintenance.

The high vacuum requirement intrinsic to most mass spectrometers is relaxed in ion trap-based instruments. By further reducing the dimensions of the ion trap to <1 mm mass spectrometry (MS) at pressures as high as 10 torr can be performed while simultaneously decreasing the volume required. This ability to operate at higher pressures (relative to other MS platforms) eliminates the need for expensive, large, power-hungry, and highly fragile turbo and rough vacuum pumps. Pressures of 1 torr can be readily achieved with low-power scroll pumps.

MS Schematic

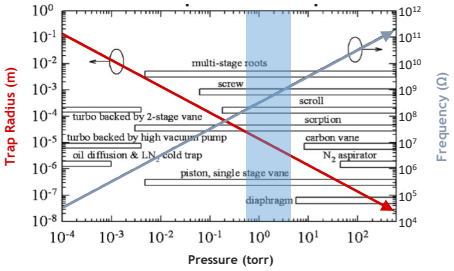


USPTO 8,878,127 Miniature charged particle trap

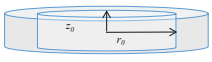
Fast-Switching Dual-Polarity APCI

The improved handheld HPMS technology shown here offers dual polarity detection over a broad mass range (m/z ~50-460). Both positive and negative mode spectra are collected in ~100 ms, which translates into multiple positive and negative mode scans across a single sample. The increased information content per scan not only improves the confidence in a target list match, but it enables the instrument to detect across the broad range of potential threats without the need to collect a second sample or pause the analysis to switch polarities.

Ion-Trap Trade-Space



Ring Electrode Schematic



Ω Ion trap radio frequency (Hz)
V_{max} operating peak voltage
q_{max} 0.908

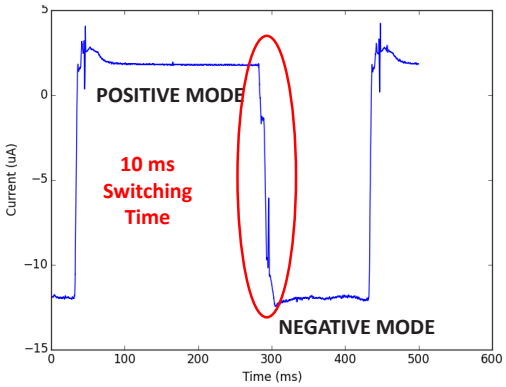
Mass Range

$$\left(\frac{m}{e}\right)_{max} = \frac{8V_{max}}{q_{max}\Omega^2(r_0^2 + 2z_0^2)}$$

Mass Resolution

$$\frac{\Delta m}{m} \propto \frac{2\sqrt{3}c}{\Omega}$$

High Voltage Power Supply (HVPS) Switching Time



908devices

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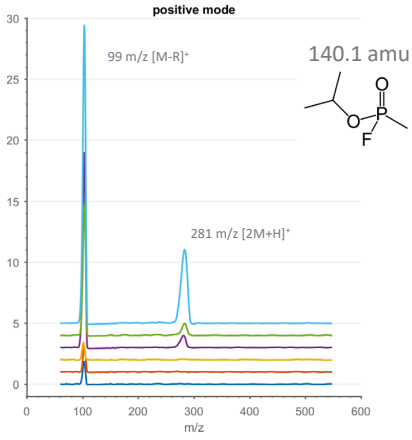
CLASSES	SUBCLASSES	EXEMPLAR TARGETS	DEVICE CAPABILITY
Chemical Warfare Agents (CWAs)	Nerve	G and V series	
	Blister	HD, L	
Toxic Industrial Chemicals (TICs)	Toxic Gases	cyanides, chlorine, phosgene, sulfur dioxide	
	Toxic Liquids	BTEX, HCl, chloroform	
	Pesticides	organophosphates/chlorines, carbamates, pyrethroids	
	Fumigants	methyl bromide, phosphine, formaldehyde	
	Refrigerants	HFCs, HCFCs	
	Fire Safety Standards	PAHs	
Explosives	Nitroaromatics	TNT, tetryl	
	Nitramines & Nitrate Esters	RDX, PETN, HMX, EGDN, NG, Semtex, Detasheet, C-4	
	Inorganic Nitrates	UN, AN, black powder, nitric acid	
	Chlorate/Perchlorate	$KClO_3$, $KClO_4$, $NaClO_3$, $NaClO_4$	
	Peroxides	TATP, HMTD, MEKP	
Drugs of Abuse	Stimulants	cocaine, amphetamine, MDMA	
	Depressants	barbiturates, GHB	
	Hallucinogens	LSD, psilocybin, dimethyltryptamine	
	Opioids	heroin, codeine, morphine, fentanyl, oxycodone	
	Cannabis	marijuana related products	
	New Psychoactive Substances	synthetic cannabinoids/cathinones, ketamine, khat	

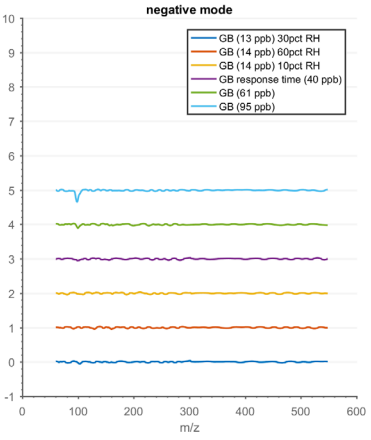
BB Demo | Limited Data/TBD | Not Detected

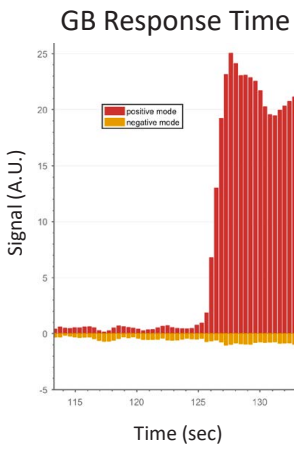
Example: Chemical Warfare Agents

The vapor sensitivity of the next-generation HPMS device lies at the low parts-per billion by volume (ppbv) level with response times on the order of a few seconds. Below is an example of direct vapor detection of Sarin (GB) and thermal desorption of VX residue.

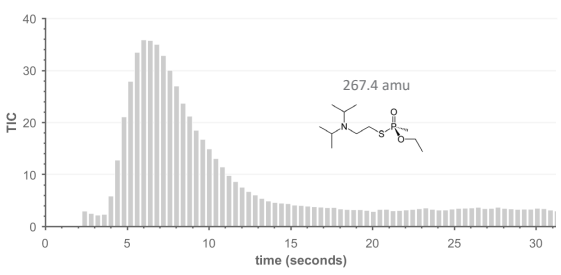
Sarin (GB) Direct Vapor Analysis

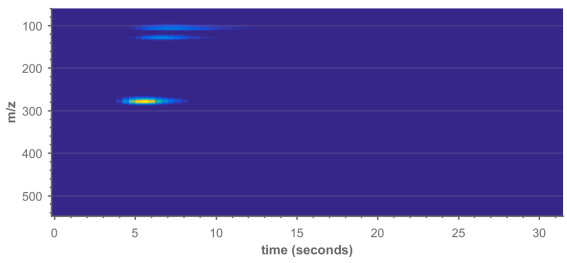


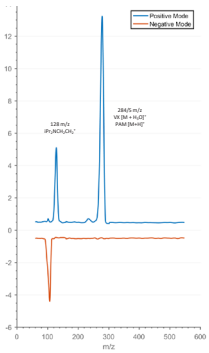




VX Thermal Desorption







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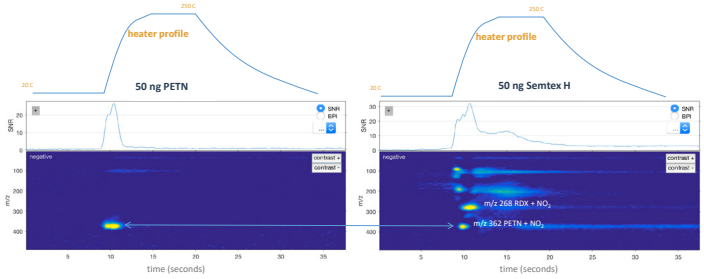
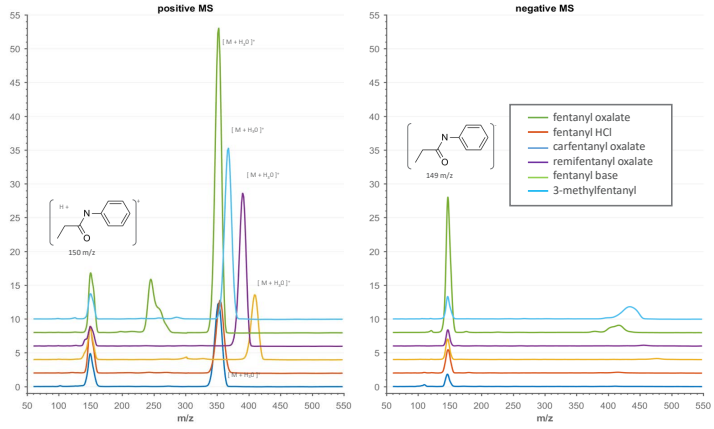
Example: Explosive Residues

Negative mode MS enables the detection of several organonitrate and some inorganic explosive compounds. An integrated thermal desorber provides controlled heating of a sample collected on a swab. Trace (<500 ng) detection of pure PETN as well as detection of both PETN and RDX in a Semtex H formulation is shown below.

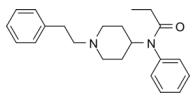


Example: Narcotics / Drugs of Abuse

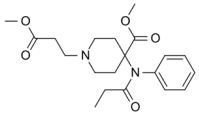
Expanded drug detection capabilities at mass loads <50 ng currently include cocaine, heroin, fentanyl and its derivatives (see below), MDMA, amphetamine, methamphetamine, cathinone, ephedrine, pseudoephedrine, norpseudoephedrine HCl, LSD, GHB sodium salt, oxycodone and PCP. Here is one example of the specificity that can be achieved with a single compound."



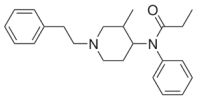
fentanyl (336.5 amu)



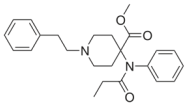
remifentanyl (376.5 amu)



3-methylfentanyl (350.5 amu)



carfentanyl (394.5 amu)



Conclusions

The fast-switching, dual-polarity of this next-generation HPMS device, offers true trace detection capabilities in both vapor (LODs in the 10s of ppbv) and thermal desorption (LODs ~10s of ng on swab) modes. This platform is a comprehensive multi-mission solution that analyzes chemical warfare agents (CWA), the full range of explosives, high priority drugs, and relevant precursors on a single sample.

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