



# Applications



## > Illicit Substances:

Explosives, CWAs and TICs:  
detection and identification at pptv-levels

### HOMELAND SECURITY THREATS

Explosives, Chemical Warfare Agents (CWA) and Toxic Industrial Compounds (TIC) are serious threats in today's global world.

The prevention of accidents or terrorist attacks involving dangerous substances is given high priority in national and international defense strategies.

Therefore the detection of small amounts of illicit substances in real-time is of utmost importance to protect citizens.

However, not only the detection of hazards is what is aimed for but also the unambiguous identification of potentially dangerous substances and for both cases the elimination of false positives or negatives is key to keeping the public safe and minimizing potential threats.

### THE SOLUTION

The IONICON PTR-MS technology allows for high-resolution monitoring and detection of compounds in gas or liquid phase present at very low concentrations.

Our solutions operate in real-time and at the same time reach a detection limit < 1 pptv. Provisional identification is possible with our high-resolution time of flight instruments.

## PTR-MS

- > Real-time ultra-sensitive VOC detection
- > Single-digit pptv-level sensitivity
- > Mass resolution up to 8000 m/Δm (FWHM)
- > Response time < 100 ms

Find out more:

[www.PTRMS.com/applications](http://www.PTRMS.com/applications)



## DETECTION OF EXPLOSIVES AND CWAs WITH PTR-MS

We conducted several experiments using different IONICON PTR-MS instruments, i.e. the High-Sensitivity PTR-MS from our PTR-QMS series which is the flagship quadrupole MS product and known for its ultra-low online detection limits of < 1 pptv, as well as the PTR-TOF 8000 from our PTR-TOFMS series featuring a mass resolution of up to 8000  $m/\Delta m$ .

Both instruments were operated using our new PTR+SRI-MS (Switchable Reagent Ions) technology enabling the use of  $H_3O^+$  or alternatively  $NO^+$  and  $O_2^+$  as precursor ions for the very efficient and soft chemical ionization in our mass spectrometers.

## RESULTS

We tested different explosives like TNT, RDX, PETN and HMX and could easily detect and identify these compounds (Fig. 1&3).

As an example of a CWA we measured mustard gas which can also be quantified in very low concentrations (Fig. 2).

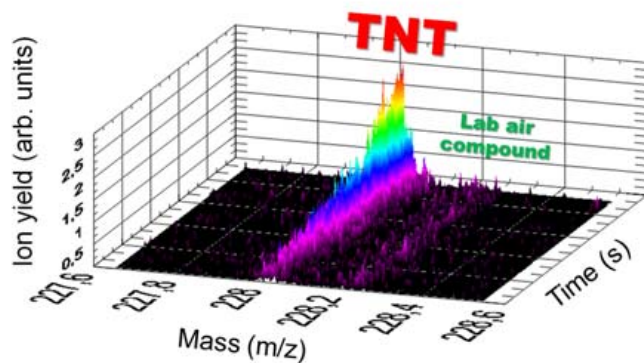


Fig. 1: Measurement of the explosive TNT with a PTR-TOF 8000 instrument. The high mass resolution guarantees that TNT on protonated mass 228.025 $m/z$  can be clearly separated from a harmless lab-air compound on the same nominal mass at 228.22 $m/z$ .

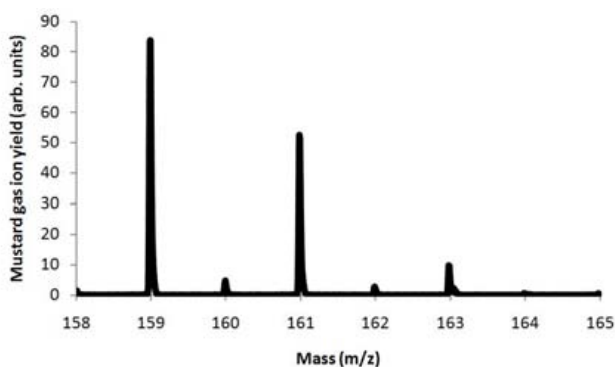


Fig. 2: The chemical warfare agent mustard gas can be identified via the exact mass in combination with its isotope ratios.

### Related articles in press:

C.A. Mayhew et al.: Applications of proton transfer reaction time-of-flight mass spectrometry for the sensitive and rapid real-time detection of solid high explosives, *International Journal of Mass Spectrometry* 289 (2010), 58–63.  
F. Petersson et al.: Real-time trace detection and identification of chemical warfare agent simulants using recent advances in proton transfer reaction time-of-flight mass spectrometry, *Rapid Commun. Mass Spectrom.* 23 (2009), 3875–3880.

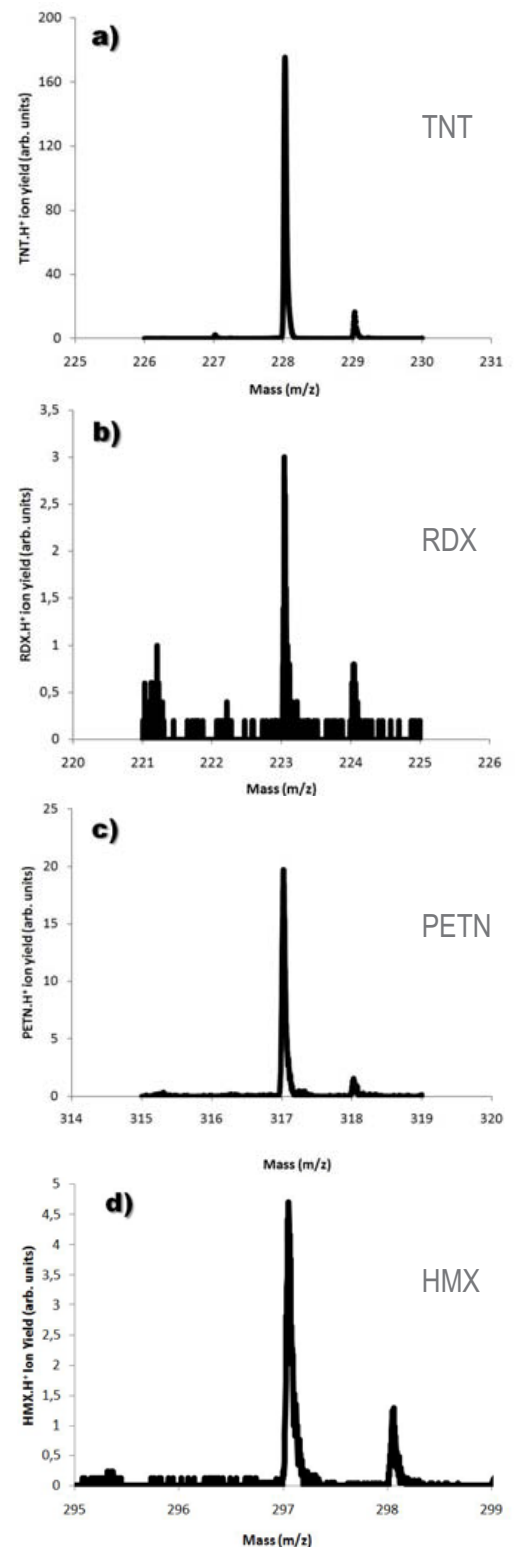


Fig. 3: The outstanding sensitivities of the PTR-TOFMS instruments make it possible to detect and identify all common solid explosives a) TNT, b) RDX, c) PETN, d) HMX) at room temperature and on a few seconds timescale.