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RESEARCH MEASUREMENT INSTRUMENTS

Application Note

Determination of TATP (triacetone triperoxide)

with Griffin 450 Mobile GC/MS/MS System Based on Cylindrical Ion Trap and with Portable X-Sorber

2011

PURPOSE OF EXPERIMENT

The purpose of the experiment was to test capabilities of the Griffin 450 mobile GC/MS/MS system with portable X-Sorber design for the collection and desorption of vapor samples for detection trace concentration of TATP after explosion.

This detection is with regard to its high volatility and its absence of detection ingredient (marker, taggant) one of the main problem in so-called „post blast“ analysis. Due to its simple preparation and sufficient explosive performance it had been considered for use as a primary charge for detonators. The reason why it has not been implemented industrially is its high volatility and low melting point. Although TATP has found neither industrial nor military applications, it has become very popular among the general public. On top of being very popular among young "scientists", this substance has also attracted attention of criminals, extremists and terrorists who use it for preparing detonators as well as main charges. TATP has been used by terrorists in many bomb attacks around the world and TATP is suicide bombers´ weapon of choice too. Experiment proved ability to detect trace concentration of TATP after explosion and instability post blast traces of TATP in time.

INTRODUCTION

TATP (triacetone triperoxide, acetone peroxide, TCAP, tri-cyclic acetone peroxide, $C_9H_{18}O_6$) is organic peroxide and a primary high explosive. It takes the form of colorless crystalline powder with a distinctive acrid odor which appears white when finely ground. Its crystal density is 1.272 $g.cm^{-3}$ (X-ray); melting point is reported in the range 95 to 98.8℃ and decomposition above 150-160℃. The heat of formation of TATP is 90.8 $kJ.mol^{-1}$. Triacetone triperoxide is non-hygroscopic and very volatile. It spontaneously recrystallizes. It is not easily soluble in water.

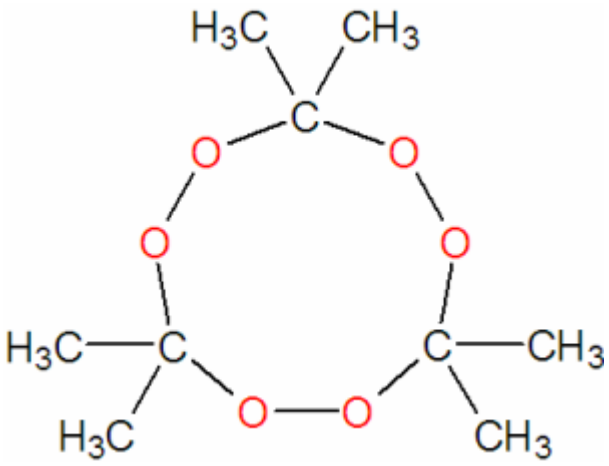

Figure 1. Chemical structure of TATP

TATP is relatively easy to make and has been used in various terrorist acts. TATP can be easily prepared in a basement lab using commercially available starting materials obtained from, e.g., hardware stores, pharmacies, and stores selling cosmetics. TATP is one of the most sensitive explosives known, being extremely sensitive to impact, temperature change and friction.
Because of the wide range of energetic materials and the many differences in their physical properties, several detection devices detect only certain types of explosives and fail to detect others. TATP is different from traditional explosive because it does not contain nitro group. Many detection devices readily detect conventional explosives made of organic nitro and nitrate compounds, but fail to detect TATP. It is almost undetectable by sniffer dogs or conventional bomb detection systems.

DESCRIPTION OF EQUIPMENT AND MEASUREMENT

Measurement was performed with the Griffin 450 mobile GC/MS/MS system based on a cylindrical ion trap mass spectrometer and with portable X-Sorber. The system was designed for mobile applications with GPS-enabled portable sampling technology and X-sorber was designed for the collection and desorption of vapor samples. This handheld collection system is compatible with Griffin 450 Mobile GC/MS/MS system.

Basic specifications:

Griffin 450	size: 48.8 cm x 48.8 cm x 53.6 cm	weight: 43.5 kg
X-Sorber	size: 21.6 cm x 16.5 cm x 7.6 cm	weight: 1.4 kg

The Griffin 450 is equipped with innovation technologies and shock mounting with additional applications including mobile labs, site monitoring and forensic analysis. And it is placed in a reinforced, ruggedized aluminium case for enhanced portability.

Figure 2. Griffin 450 with X-Sorber and laptop displaying Griffin System Software

The X-Sorber is easy to operate weighing only 1.4 kg. Battery operated with up to 12 hours sample time and rechargeable when is docked with Griffin 450. The X-Sorber contains two durable stainless steel sorbent tubes with unique serial numbers, which are re-usable and compatible with other commercial thermal desorbers. Samples can be collected onto Tube A, Tube B, or both.

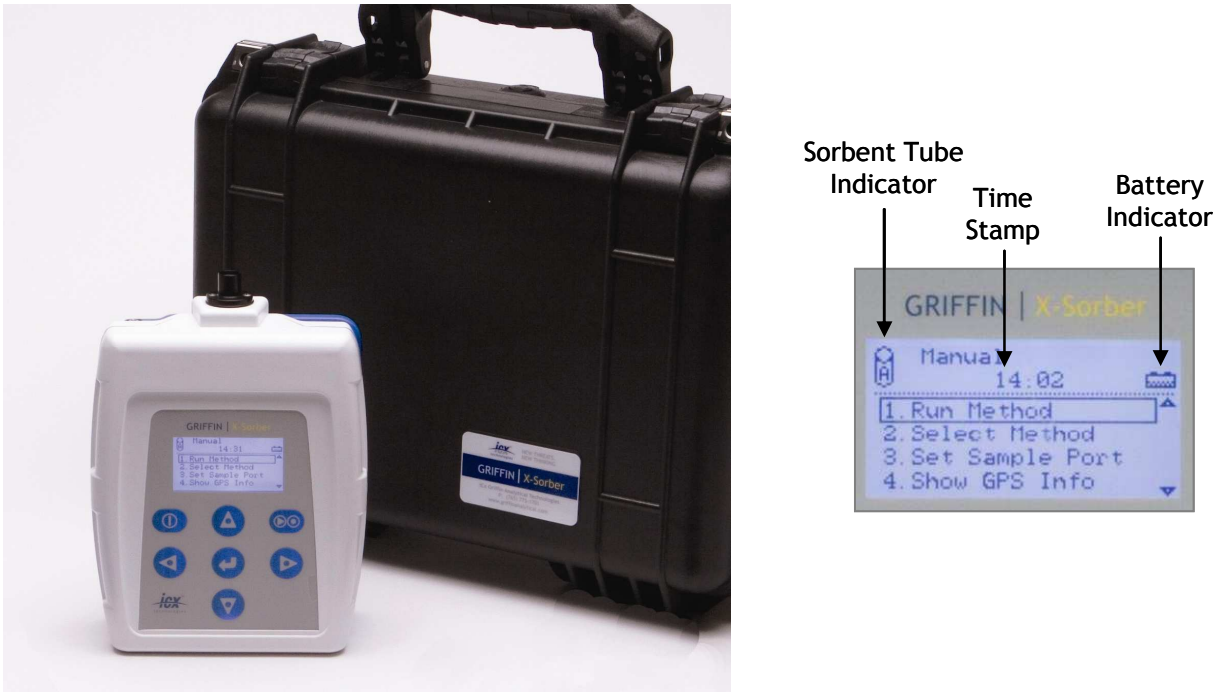

Figure 3. X-Sorber, portable vapor sampler and desorber

Sampling point post blast traces

Sampling of vapor samples of TATP was performed in area of University of Pardubice, in Institute of Energetic Materials in Doubravice.

Figure 4. Practical application sampling of post blast traces of TATP in area of University of Pardubice, Institute of Energetic Materials

Preparation of charge with TATP

The size of the charge was 40 mm in diameter (in a standard instrument) and 100 mm in height (Figure 4). The charge was filled up to density 0.45 $g.cm^{-3}$. Initiation the charge was by standard Detonator No. 8. Actual outside temperature was 23℃ and 35℃ in the sun.

Sampling

It was collected vapor sample of pure TATP before explosion (Figure 7 and 10) during time of 2 minutes (circa 1260 ml) by portable X-Sorber and then X-Sorber was docked with the Griffin 450 for data download and sample identification.

The same procedure was performed by X-sorber after 1 hour after explosion (Figure 8 and 11) and 24 hours after explosion (Figure 9 and 12).

Test of X-Sorber sorption ability

It was tested X-Sorber sorption ability in time in lab (Figure 5). Vapor samples of pure TATP were collected by X-Sorber (2 minutes, circa 1260 ml) and analyzed with the Griffin 450. Analyses were performed after 1 minutes, 1 hour, 1 day and 3 days. For each test was used a new tube which was put through cleaning process. Therefore the Griffin 450 has a second docking port which provides a conditioning station for recently sampled X-Sorber to be prepared for re-use.

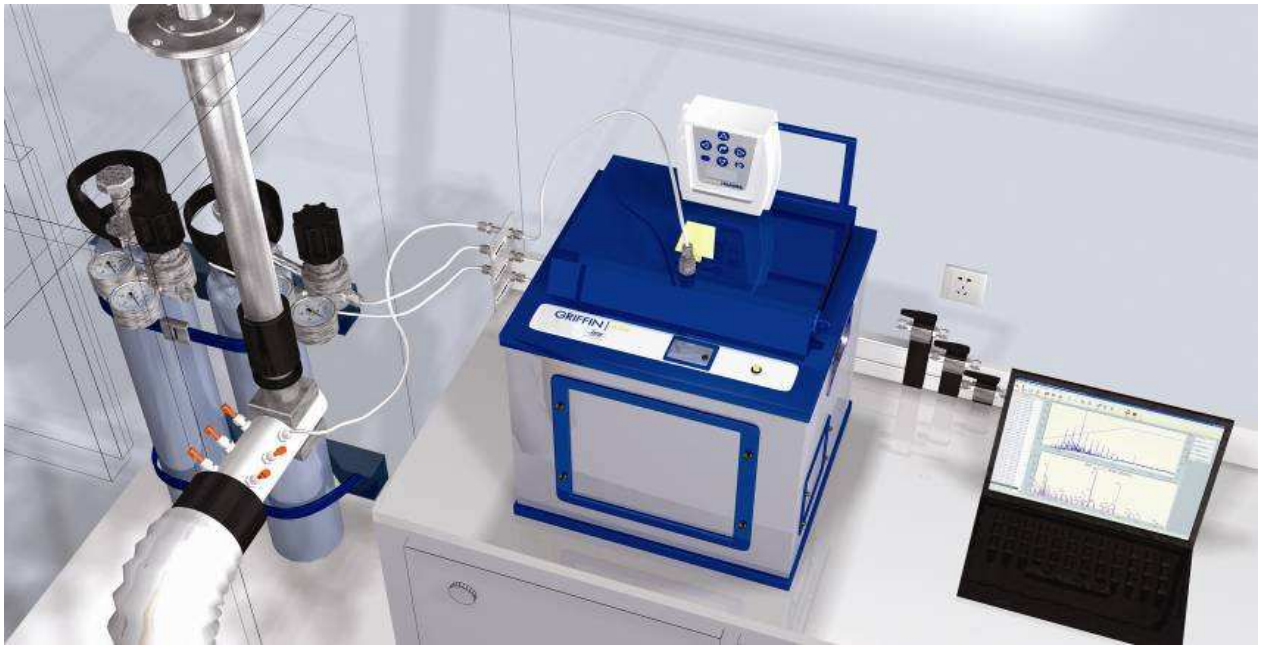

Figure 5. Griffin 450 with X-Sorber and laptop in lab

RESULTS AND DISCUSSION

Qualitative analysis (comparison of MS spectra of TATP)

The mass spectrometer was operated in full MS mode scanning over the mass range m/z 40 - 425. Comparison of mass spectrum of TATP from the Griffin 450 (top) and NIST library (bottom) is shown in Figure 6.

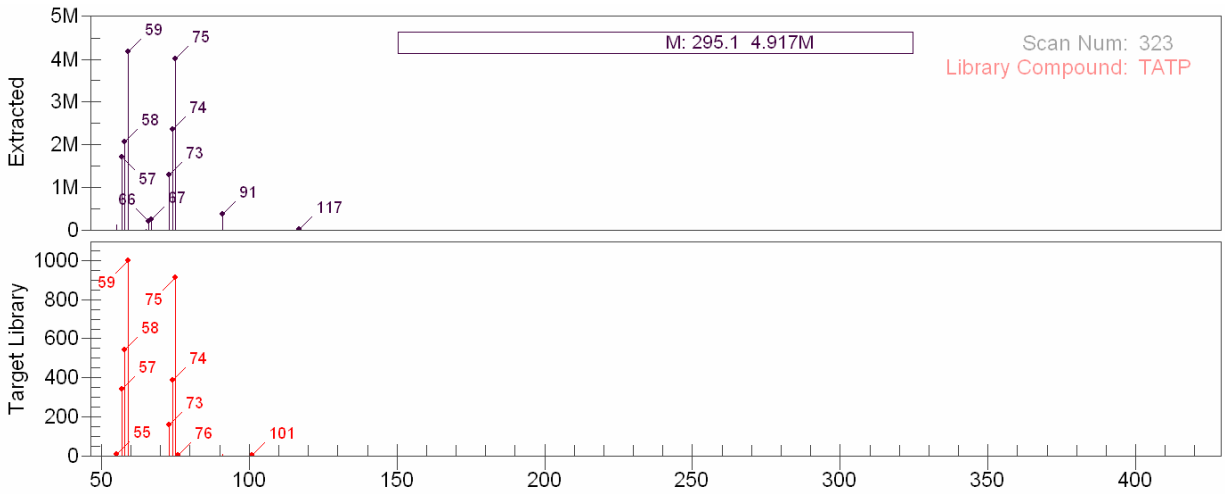

Figure 6. Comparison of mass spectra of TATP from Griffin 450 (top) and NIST library (bottom)

Semiquantitative analysis (comparison of area peak of TATP)

Result analysis of pure TATP before explosion – Area 3 771 000 cps.

Scan Number: 323
Retention Time: 2,85

Compound	GMF	Concentration
TATP	89*	n/a

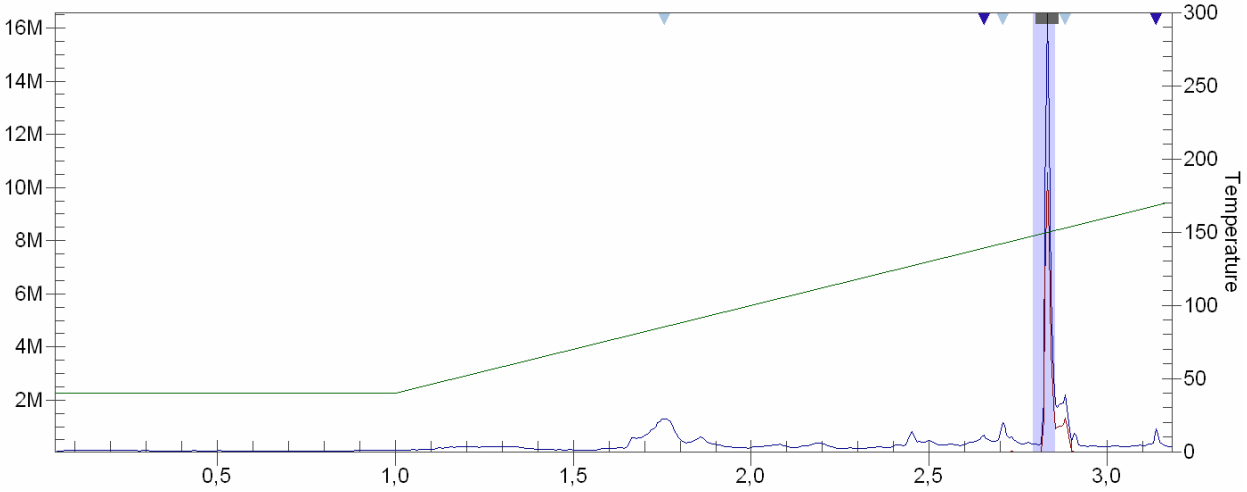

Figure 7. Analysis of pure TATP before explosion

Result analysis of TATP 1 hour after explosion – Area 610 152 cps.

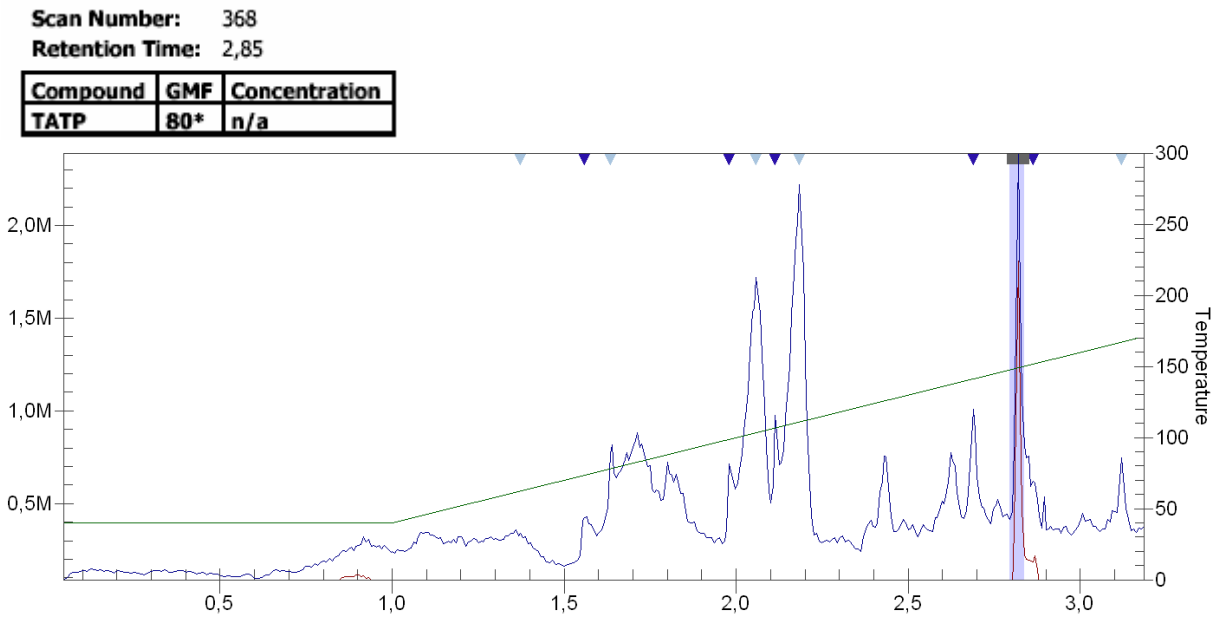

Figure 8. Analysis of TATP - 1 hour after explosion

Result analysis of TATP 24 hours after explosion – Area 0 cps, No response was identified.

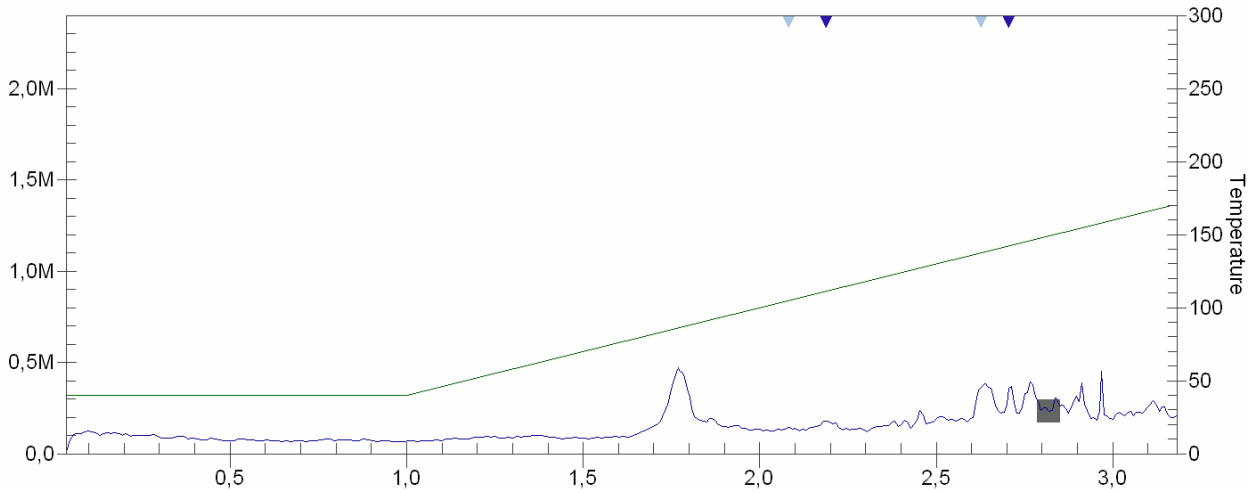

Figure 9. Analysis of TATP - 24 hours after explosion

Time	Area
0 hour	3 771 000 cps
1 hour	610 152 cps
24 hours	0 cps

Table 1. Summary of results analysis of TATP

Comparison of chromatograms of TATP (0, 1 and 24 hours)

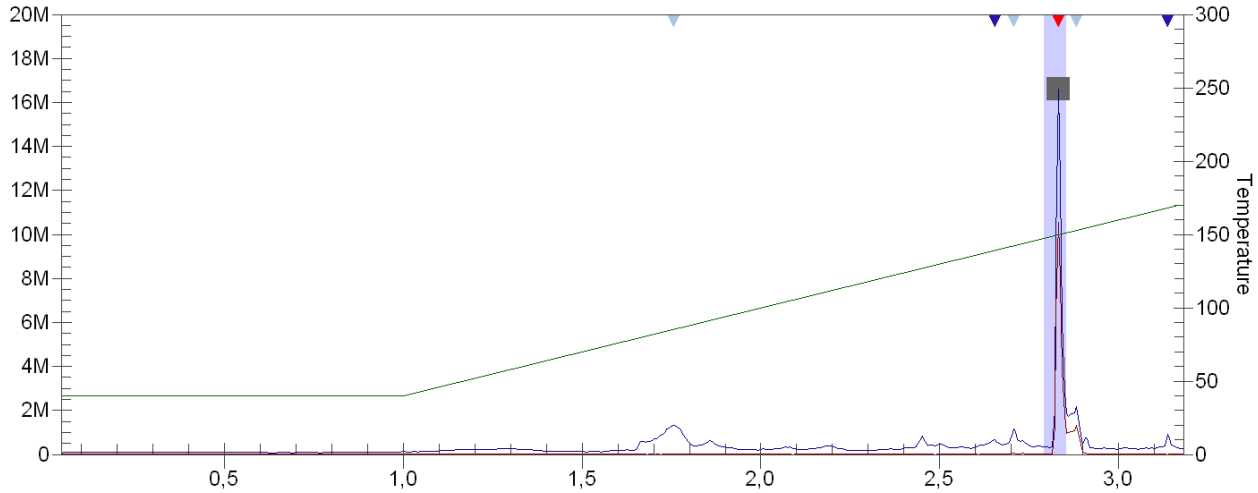

Figure 10. Analysis of pure TATP before explosion

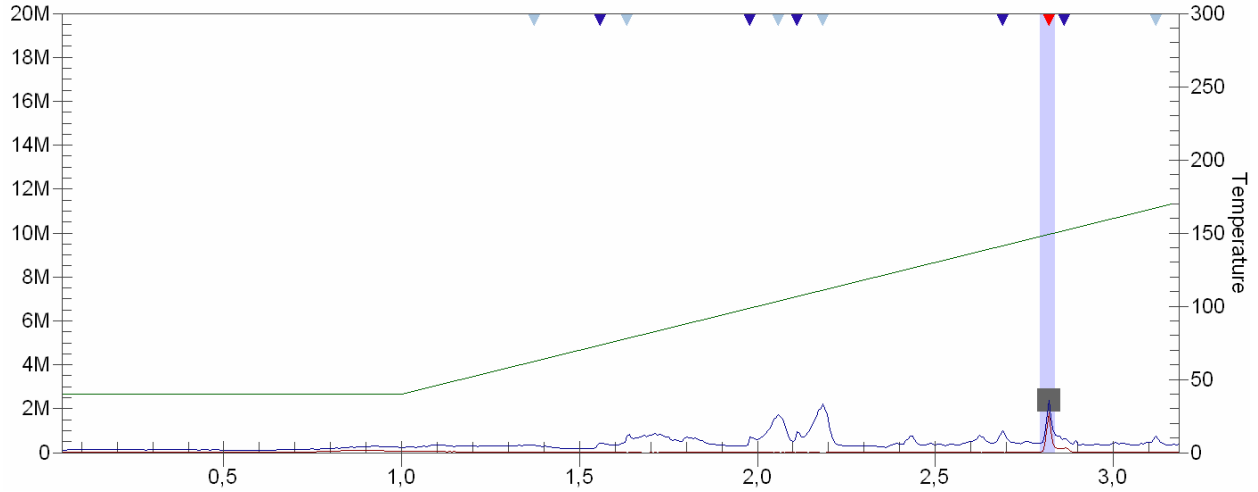

Figure 11. Analysis of TATP - 1 hour after explosion

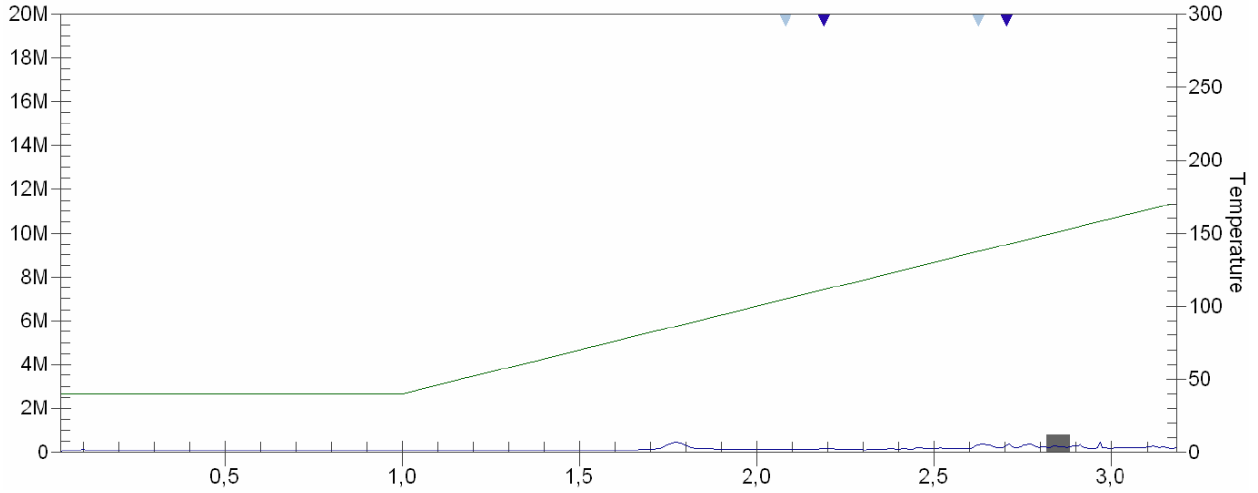

Figure 12. Analysis of TATP - 24 hours after explosion

Test of sorption ability of X-Sorber in time

Analyses were performed after 1 minutes, 1 hour, 1 day and 3 days (Table 2). Each tube was sorbed during 2 minutes (volume circa 1260 ml)

Time	Area
1 minute	3 781 000 cps
1 hour	3 693 000 cps
1 day	3 599 000 cps
3 days	3 457 000 cps

Table 2. Sorption ability of X-Sorber

CONCLUSIONS

It was proved the Griffin 450 Mobile GC/MS/MS system can be used for the detection and identification of traces TATP.

It was proved ability to detect trace concentration of TATP after explosion and instability post blast traces of TATP in time. Vapor samples of pure TATP were successfully collected by X-Sorber and analyzed with the Griffin 450 mobile GC/MS/MS system. The method requires no sample preparation and results of analysis are in just minutes.

Results of measurement showing very good detection both direct pure TATP and traces of TATP after explosion. And it was found out the detection is with regard to its high volatility is insignificant, because it was found no traces after 24 hours after explosion. It means that detection after explosion on site must be as fastest as possible.

It was successfully tested sorption ability of X-Sorber in time. The vapor sample which was analyzed immediately or after 3 days showed the similar results.