

APPLICATIONS

Analytical Approaches for the Identification and Quantitation of Organic Explosives by LC-HRMS

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Introduction

Sensitive and accurate determination of explosive materials is important for crime scene investigations and to address potential safety concerns within geographical warzones. Traditional GC and HPLC based methods are often cumbersome with lengthy run-times, limited specificity, sometimes relying on dual methods for confirmation.

Here we describe a high resolution mass spectrometry (HRMS) analytical method with fast run-times and increased confidence for organic explosive identification.

Experimental Conditions

LC-MS/MS Conditions

6.5 min Method

Column: Luna® Omega 3 µm Polar C18

Dimensions: 100 x 3.0 mm

Part No.: OOD-4760-Y0

Mobile Phase: A: Aqueous Buffer*

B: Methanol/Acetonitrile

Injection: 7 µL

HPLC System: SCIEX ExionLC™ AC

2.5 min Method

Column: Synergi™ 2.5 µm Hydro-RP

Dimensions: 20 x 2.0 mm, MercuryMS™

Part No.: OOM-4387-B0-CE

Mobile Phase: A: Aqueous Buffer*

B: Methanol/Acetonitrile

Injection: 7 µL

HPLC System: SCIEX ExionLC AC

Detector

Ion Source: Turbo V™ with Twin Sprayer APCI Probe

Mass Analyzer: SCIEX X500R QTOF System

Acquisition: SWATH® and MRMHR workflow with SCIEX OS software 1.3

* Detailed mobile phase, gradient, and flow conditions available from Phenomenex and SCIEX.

Figure 1.
6.5 min method

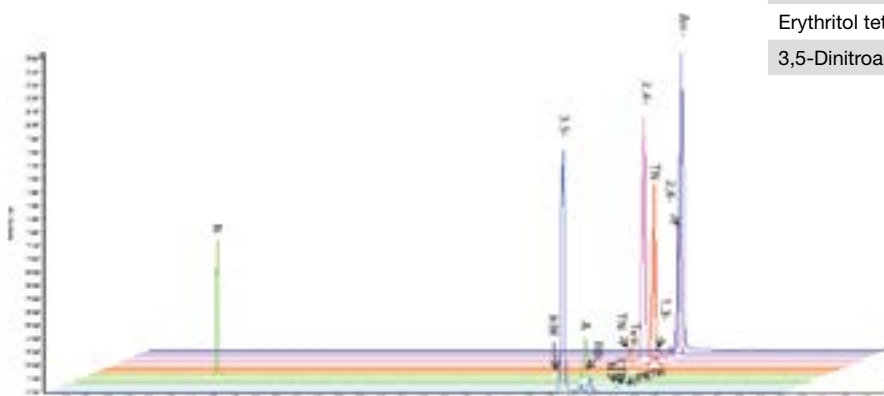


Figure 2.
2.5 min method

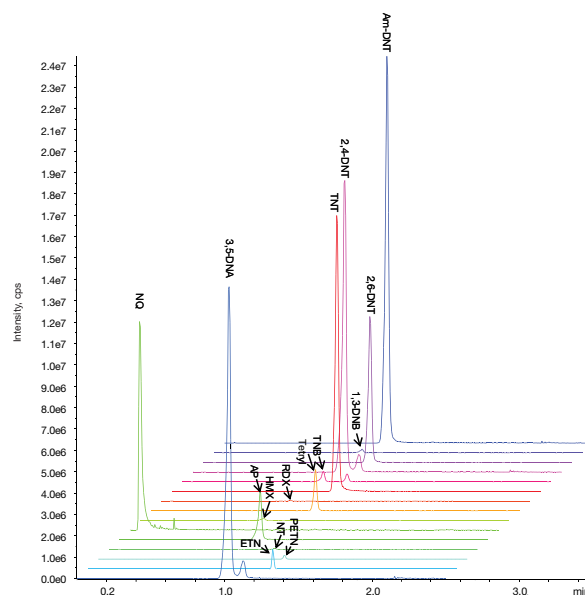


Table 1.
Organic Explosive Compounds List

| Analyte | Abbreviation |
|---|--------------|
| Nitroguanidine | NQ |
| Ammonium Picrate | AP |
| Octahydro-1,3,5,7-tetranitro-1,3,5,7-triazine | HMX |
| Hexahydro-1,3,5-trinitro-1,3,5-triazine | RDX |
| 1,3,5-Trinitrobenzene | TNB |
| 1,3-Dinitrobenzene | 1,3-DNB |
| 2,4,6,N-tetranitro-N-methylaniline | Tetryl |
| 2,4,6-trinitrotoluene | TNT |
| 4-Amino-4,6-dinitrotoluene | Am-DNT |
| 2,6-Dinitrotoluene | 2,6-DNT |
| 2,4-Dinitrotoluene | 2,4-DNT |
| Pentaerythritol tetranitrate | PETN |
| Erythritol tetranitrate | ETN |
| 3,5-Dinitroaniline | 3,5-DNA |

APPLICATIONS

Conclusion

Luna[®] Omega 3 μ m Polar C18 100 x 3.0 mm column provided very high HPLC performance with excellent selectivity for organic explosives with a LC run-time of 6.5 minutes, while Synergi[™] 2.5 μ m Hydro-RP provided a good alternative fast LC run-time of 2.5 minutes in a MercuryMS[™] 20 x 2.0 mm cartridge format.

These methods applied with the SCIEX X500R QTOF System provides the speed and mass accuracy for the high-throughput identification and quantitation of organic explosives in forensic analytical settings.

Luna Omega Ordering Information

| 3 μ m Minibore Columns (mm) | | | | | SecurityGuard [™] Cartridges (mm) |
|---------------------------------|-------------|-------------|-------------|-------------|---|
| Phases | 30 x 2.1 | 50 x 2.1 | 100 x 2.1 | 150 x 2.1 | 4 x 2.0* (10/pk) |
| Polar C18 | 00A-4760-AN | 00B-4760-AN | 00D-4760-AN | 00F-4760-AN | AJO-7600 |
| | | | | | for ID: 2.0 - 3.0 mm |

| 3 μ m MidBore [™] Columns (mm) | | | | SecurityGuard [™] Cartridges (mm) |
|---|-------------|-------------|-------------|---|
| Phases | 50 x 3.0 | 100 x 3.0 | 150 x 3.0 | 4 x 2.0* (10/pk) |
| Polar C18 | 00B-4760-YO | 00D-4760-YO | 00F-4760-YO | AJO-7600 |
| | | | | for ID: 2.0 - 3.0 mm |

| 3 μ m Analytical Columns (mm) | | | | | SecurityGuard [™] Cartridges (mm) |
|-----------------------------------|-------------|-------------|-------------|-------------|---|
| Phases | 50 x 4.6 | 100 x 4.6 | 150 x 4.6 | 250 x 4.6 | 4 x 3.0* (10/pk) |
| Polar C18 | 00B-4760-E0 | 00D-4760-E0 | 00F-4760-E0 | 00G-4760-E0 | AJO-7601 |
| | | | | | for ID: 3.2-8.0 mm |

* SecurityGuard[™] Analytical Cartridges require holder, Part No.: KJO-4282

Synergi Hydro-RP HPLC Columns

| 2.5 μ m MercuryMS LC/MS Cartridges (mm) | | | |
|---|----------------|----------------|----------------|
| Phases | 10 x 2.0 | 10 x 4.0 | 20 x 2.0 |
| Hydro-RP | 00N-4387-B0-CE | 00N-4387-D0-CE | 00M-4387-B0-CE |



If Phenomenex products in this technical note do not provide at least an equivalent separation as compared to other products of the same phase and dimension, return the product with comparative data within 45 days for a FULL REFUND.

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Disclaimer

Comparative separations may not be representative of all applications.

SecurityGuard is patented by Phenomenex. U.S. Patent No. 6,162,362

CAUTION: this patent only applies to the analytical-sized guard cartridge holder, and does not apply to SemiPrep, PREP or ULTRA holders, or to any cartridges.

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