B51 Optimization Parameters of Fragmentary Voltage and Collision Energy for the Identification and Separation of 1,3,5-Triamino-2,4,6-Trinitrobenzene (TATB) From Other Explosives With Liquid Chromatography/Tandem Mass Spectrometry (LC/MS/MS)

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Learning Overview: After attending this presentation, attendees will better understand the development and optimization of the parameters for the creation of a new method for the identification and separation of organic explosives.

Impact on the Forensic Science Community: This presentation will impact the forensic science community by describing the current capabilities of the Kosovo legal science lab in the development of new methods for the identification and separation of organic explosives by chromatographic methods and the impact on the identification of source(s) explosives and interconnections to identify terrorists.

Explosives are classified in several ways, based on different criteria. Thus, explosives are divided into high and low explosives based on the type and speed of the action. Explosives are also classified according to their chemical structure. The most important group is that of organic compounds containing the nitro (NO_2) group. They are further subdivided based on the site where NO_2 is attached to the atomic structure. Nitrogen compounds contain C-NO_2 groups, a group of C-O-NO_2 nitrate ethers, and C-N-NO_2 nitrite nitriles.

There are different methods for identifying and separating organic explosives, especially 1,3,5-triamino-2,4,6-trinitrobenzene (TATB), but recently, double-mass spectrometric detector chromatography has begun to accommodate numerous scientific researches by forensic scientists to find appropriate parameters for the identification and separation of organic explosives in low concentrations in picograms (pg) or even in femtograms (fg).

Therefore, considering the needs, reasonable work has begun to create optimal parameters for Collision Energy (CE) and Fragmentary Voltage (FV) for identifying and dividing TATB from other explosives by using LC/MS/MS with the Atmospheric Pressure Chemical Ionization (APCI) model, Zorbox® SB–C18 column 600 bar 3 x 50mm 3.5µm and mobile phase methanol/isopropanol/water (1:3:6), as well as 0.1% chloroform.

In studying this, optimal CE and FV values have been established for the identification and separation of TATB from other explosives, the change of fractional energy values greatly influences the fragmentation of the molecule under study, the fragmentation fractions molecule at all levels, and this facilitates the identification of the molecule of the unknown explosive, and all fractions comply with the preliminary knowledge of the TATB structure and knowledge of its potential fragmentation, in addition to the excellent division achieved with this technique and the limit of detection down to fg.

At the end of this study, optimized parameters for identification and separation of organic explosives with LC/MS/MS result in the following conclusions. This study analyzed the following organic explosive samples: 3,4,8,9,12,13-Hexaoxa-1,6-diazabicyclo(4.4.4)tetradecane (HMTD), 1,3,5,7-Tetranitro-1,3,5,7-tetrazocane (HMX), RDX, TATB, 1,2-dinitroxyethane (EGDN), 1,3,5-Trinitrobenzene (1,3,5-TNB), 1,3-Dinitrobenzene (1,3-DNB), *N*-Methyl-*N*-(2,4,6-trinitrophenyl)nitramide (TETRYL), 4-amino-2,6-dinitrotoluene (4A-DNT), Nitrobenzene (NB), Nitroglycerin (NG), 2-amino-2,6-dinitrotoluene (2A-DNT), 2,4,6-Trinitrotoluene (TNT), 2,6-Dinitrotoluene (2,6-DNT), 2,4-Dinitrotoluene (2,4-DNT), 1,3,5-Trinitro-2-[2-(2,4,6-trinitrophenyl)ethenyl]benzene (HNS), 2-Nitrotoluene (2-NT), 4-Nitrotoluene (4-NT), 2,2-Bis[(nitrooxy)methyl]propane-1,3-diyl dinitrate (PETN), 3-Nitrotoluene (3-NT), 3,3-Dimethyl-1,2-dioxacyclopropane (TATP), and CARBAMITE. This work allowed the creation of methods for the identification and separation of explosives doing the optimization of parameters on LC and MS/MS.

During the study, methods for specific explosives were created: HMX, RDX, TATB, TETRYL, TNT, 2,6-DNT, HNS, PETN, and CARBAMITE. These were named: (1) EKSPLOSIVES-MMI-APCI.m, and (2) EKSPLOSIVES _2-6-2-4_DNT_MMI-APCI.m.

Parameter optimization for both methods was accomplished as follows: flow of mobile phase was 0.5mL/minute, temperature of column was 35°C, and the length of column was 3x50mm, the diameter was 3.5µm, the Ionization source Multimode (MMI), ionization model (APCI), and volume of sample injected was 20µm. Mobile phase was suitable for both above methods.

Optimization of parameters was conducted as FV and CE for the explosives listed above to identify and separate explosives in a trace amount at the fg level.

TATB, Collision Energy, LC/MS/MS

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