B98 Optimization Parameters of Fragmentary Voltage and Collision Energy for the Identification and Separation of N-Methyl-N-(2,4,6-Trinitrophenyl)nitramide (TETRYL) From Other Explosives With Liquid Chromatography/Tandem Mass Spectrometry (LC/MS/MS)

Milazim Tahirukaj, Kosovo Agency on Forensic, Pristina, Kosovo 10000, KOSOVO; Blerim Olluri, PhD*, Bill Clinton, Prishtina 10000, KOSOVO; Andriana Surleva, University of Chemical Technology and Metallurgy, Sofia, BULGARIA; Herolind Krasniqi*, Kosovo Agency on Forensic, Pristina 10000, KOSOVO; Xhemajl Ademaj, PhD*, Lawyer Office, Prishtina 10000, KOSOVO; Nedzad Korajlic, PhD, Sarajevo 71000, BOSNIA AND HERZEGOVINA*

Learning Overview: After attending this presentation, attendees will better understand the Kosovo Agency for Forensic Achievements 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 a 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, the explosives are divided into: high and low explosives based on the type and speed of the action they are doing. 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 TETRYL, 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 pictograms (pg) or even in fentograms (fg).

Therefore, considering the needs reasonable we have begun to create optimal parameters for Collision Energy (CE) and Fragmentary Voltage (FV) for identifying and dividing TETRYL from other explosives by using the 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.

Studies have found optimal CE and FV values for the identification and separation of TETRYL from other explosives, the change of fractional energy values greatly influences the fragmentation of the molecule being studied, and the fragmentation fractions molecule at all levels. This facilitates the identification of the molecule of unknown explosive and all fractions comply with the preliminary knowledge of the TETRYL structure and knowledge of its potential fragmentation, in addition to the excellent division achieved with this technique and the limit of detection up 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. In this study, the samples analyzed were organic explosives: 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, 1,3,5-Triamino-2,4,6-Trinitrobenzene (TATB), 1,2-Dinitroxyethane (EGDN), 1,3,5-Trinitrobenzene, 1,3-DNB (1,3-Dinitrobenzene (1,3,5-TNB), 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-Nitrotolueni (2-NT), 4-Nitrotolueni (4-NT), 2,2-Bis[(Nitrooxy)Methyl]Propane-1,3-Diyl Dinitrate (PETN), 3-Nitrotolueni (3-NT), 3,3-Dimethyl-1,2-Dioxacyclopropane (TATP), and Carbamite; the creation of methods for identification and separation of explosives by doing the optimization of parameters on LC and MS/MS.

This study attempted to create methods just for explosives like HMX, RDX, TATB, TETRYL, TNT, 2,6-DNT, HNS, PETN and carbamite. The two methods created are: EKSPLOSIVES-MMI-APCI.m and EKSPLOSIVES _2-6-2-4_DNT_MMI-APCI.m.

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

For the above explosives, this study has conducted optimization of parameters as FV and CE for the identification and separation of explosives in a trace amount until fg.

TETRYL, Collision Energy, Fragmentary Voltage

*Presenting Author