B87 LC/MS of Explosives: RDX Characterization Through Impurity Profiles

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The objective of this paper is to present the forensic community a methodology for characterization of a common explosive, RDX.

This study provides the tools for a methodology to detect trace components, such as byproducts, precursors, degradation products and additives in RDX, thus providing an individualizing profile or a fingerprint for a particular explosive sample. Accordingly, such a profile, when finally developed, may be of a great value in differentiating and sourcing samples.

Type and origin of an explosive is one the most important questions to be addressed in a bombing investigation. RDX (1,3,5-trinitro-1,3,5triazacyclohexane) is a high power explosive that is extensively used for military and commercial applications throughout the world. Unlike TNT, RDX does not have isomers that may serve as markers for profiling. Furthermore, many precursors and intermediates do not seem to survive harsh manufacturing conditions.

Liquid chromatography - mass spectrometry (LC/MS) is an attractive technique for the analysis of trace levels of explosives because the analyses are conducted at room temperature thus preserving thermally labile compounds. This paper reports a study for the characterization of RDX through its impurities and degradation products profile using LC/MS. This study will give forensic scientists the tools for the development of a method to determine the manufacturing route and to estimate time of manufacture. In addition to HMX that is the major impurity in RDX, seven other compounds were found in RDX samples. They can be divided in three groups:

1. Acetylated nitramines; common byproducts in RDX manufac turing by the Bachman method
2. 1,3-dinitro-5-nitroso-1,3,5-triazacyclohexane; an RDX degradation product
3. Impurities not associated with a particular manufacturing method All these compounds contribute to a profile of an individual sample that might lead to a fingerprint or a signature of that sample. It also can be seen as a future tool that will facilitate relation of the sample to its probable source due to some impurities being specific to a particular manufacturing route. Degradation products and other impurities may accumulate as the sample is exposed to the environment and therefore their concentration could be used as a measure of the sample age.

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