B17 Forensic Analysis of Illicit Drugs by Nitrogen Direct Analysis in Real-Time Mass Spectrometry (N_2 DART®-MS)

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After attending this presentation, attendees will appreciate a new mode of DART®/MS using cheaper and more easily accessible N_2 instead of the popularly used Helium (He) as the DART® ionization gas, its great ionization capabilities for illicit drugs, and a general analytical protocol to use N_2 DART®/MS for the forensic analysis of illicit drugs with either a JEOL AccuTOF™ orthogonal Time-Of-Flight (TOF) MS or an Agilent® 6550 quadrupole TOF (qTOF) MS.

This presentation will impact the forensic science community by introducing a novel N_2 DART®/MS technique to effectively ionize seized drug evidence, which has the potential to be used with a miniature mass spectrometer in the future for the forensic analysis of illicit drugs at crime scenes.

Currently, helium gas is popularly used in DART®/MS. Theoretically, He DART®/MS should have the best sensitivity because He is an inert gas that occupies a front position in the periodic table, therefore producing metastable species with the highest internal energy (i.e., long-lived He 2^3S electronic excited state atoms with an internal energy of 19.8eV); however, when He gas is not readily available (e.g., during space missions or the forensic analysis of illicit drugs at the crime scene), nitrogen gas is the best option because it is the next inert gas behind He in the periodic table.

In this study, N_2 DART®/TOF/MS with a JEOL AccuTOF™ mass spectrometer was first used to analyze ten commonly abused drugs (i.e., (±)-amphetamine, cocaine, diazepam, heroin, Lysergic Acid Diethylamide (LSD), (±)-3,4-Methylenedioxymethamphetamine (MDMA), Phencyclidine (PCP), psilocin, testosterone, and Δ^9-Tetrahydrocannabinol (THC)) to test the ionizing capability of N_2 DART® toward compounds with diverse functional groups, optimize the instrumental conditions for forensic analysis of illicit drugs, estimate the Limit Of Detection (LOD) of the analysis, and develop a general analytical protocol for the analysis. Under optimum conditions, the LOD of N_2 DART®/TOF/MS was determined to be approximately 10μg/mL. Because the sampling volume was approximately 1μL, the LOD of N_2 DART®/TOF/MS was approximately 10pg in quantities. The general analytical protocol took approximately three minutes in the analysis of each commonly abused drug. All the commonly abused drugs were positively identified at 10μg/mL as the experimentally measured monoisotopic mass of multiple ions, predominately the $[M+H]^+$ ion, from each drug were within ±5mDa of the theoretically calculated monoisotopic mass. No time-consuming and labor-intensive sample preparation steps were required during the analysis. The general analytical protocol was then applied to the tablet analysis of six prescriptions drugs (i.e., clonazepam 1mg, cyclobenzaprine 10mg, metaxalone 800mg, oxycodone/acetaminophen 5/325mg, tramadol/APAP 37.5/325mg, and zolpidem 10mg). It was found that while N_2 DART® was able to efficiently ionize and subsequently identify the active ingredients in the tablets, it practically omitted the inactive ingredients. Therefore, it was concluded that the general analytical protocol can be utilized in the analysis of seized drugs because they are mixtures with similar complexity as the tablets.

N_2 DART®/qTOF/MS with an Agilent® 6550 mass spectrometer was further used to analyze ten commonly abused drugs at 10μg/mL in order to test the applicability of N_2 DART® on different MS platforms. First, all of the commonly abused drugs were positively identified by TOF/MS of the $[M+H]^+$ ions with their monoisotopic mass and isotopic pattern. Then, they were further positively identified by qTOF/MS/MS of the $[M+H]^+$ ions at Collision-Inducted Dissociation (CID) at 10.0V and 20.0V. The obtained mass spectra were automatically matched with the Agilent® Forensic Toxicology Personal Compound Database and Library (PCDL).

Illicit Drugs, N_2 DART®/MS, Seized Drug Analysis