

Title: Implementation of a Thermo Scientific™ Q Exactive™ Hybrid Quadrupole-Orbitrap™ Mass Spectrometer with TraceFinder™ Software for the Identification and Quantitation of Synthetic Cannabinoids in Postmortem Forensic Investigations

Presenters: Taís R Fiorentin, PhD, and Alex J Krotulski, PhD

Abstract:

Synthetic cannabinoids continue to appear in forensic toxicology casework, creating high risk scenarios for drug users as newer generations can be more potent than previous iterations. Synthetic cannabinoids represent a chemically diverse class of substances with particularly difficult behaviors to which high resolution mass spectrometry (HRMS) can provide great benefit. To better understand its toxicity and implication in forensic casework, a quantitative confirmatory test was developed and validated for 5F-MDMB-PICA (the most prevalent synthetic cannabinoid identified in forensic casework) and its metabolites in human blood. A Thermo Scientific™ Vanquish UHPLC Systems coupled with a Thermo Scientific™ Q Exactive™ Hybrid Quadrupole-Orbitrap™ Mass Spectrometer was used for analysis. Chromatographic separation was achieved using a reverse phase gradient across a Thermo Scientific™ Accucore™ Vanquish™ C18+ analytical column (100 x 2.1mm, 2.6µm). The method was quantitatively validated in accordance with ASB Standard Practices for Method Validation in Forensic Toxicology. Data was processed using Thermo Scientific™ TraceFinder™ Clinical software (Version 4.1). This interactive presentation will provide an overview of Thermo Scientific™ software, specifically with respect to its use in determining method setpoints and building a library database. Performance characteristics will be reviewed to demonstrate the utility and accuracy of the developed assay.