Testing and Quantification of a Representative Panel of Illicit Drugs in Urine and Serum Using LC-Time-of-Flight Mass Spectrometry
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1 Introduction
The panel of drug compounds used in this work are examples of commonly studied molecules in this compound class. The full list of compounds is displayed in Table 1. Immunoassays have traditionally been used for specimen testing but are well known for potential false negatives. Additionally, immunoassays are not always sensitive enough to detect low levels of drugs in challenging matrices, and can often not identify specific drugs within drug classes, due to their lack of specificity. GC/MS, which is used extensively for compounds in these classes, offers its own challenges. Many compounds are polar and often thermally labile, requiring derivatization prior to enhanced volatility. Thermally labile compounds may be misidentified due to common EI fragments with other compounds. Unlike GC/MS, LC/MS typically does not require derivatization of samples, and is ideally suited for the rapid analysis of these compounds. In 2011, guidelines were altered to allow the use of LC/MS instruments for urine quantitative confirmatory analysis. Among the LC techniques, LC/MS/MS is often used to quantitate compounds in a variety of matrices, due to its sensitivity and selectivity. However, triple quadrupole techniques can have a high cost and lack the ability to easily identify new or unknown compounds. We present an alternative workflow to test and quantify such compounds in a research setting, utilizing a rapid LC method with time-of-flight mass spectrometry (TOF).

2 Experimental
All standards were purchased from Cerilliant (Round Rock, TX).

Urine Sample Preparation: Urine was diluted 1:1 with water and directly injected, no sample extraction was required.

Urine Calibration Curves: Urine blanks were spiked with the 11 drugs in Table 1. 300 ng/mL of deuterated internal standard (IS), and then diluted 1:1 with water. The deuterated MDMA IS was used as an IS for both MDA and MDMA. Each calibration level was injected five times.

3 Results

4 Conclusion
The detection limits of the compound panel analyzed by the TOF were approximately 1.5-2.000 times lower than those required by regulatory guidelines for these types of compound, and quite adequate for research purposes. In addition to the adequate quantitative dynamic range of the AxION® 2 TOF, which rivals capabilities of the triple quadrupole instruments, TOF collects "all the ions," and provides full spectrum information which allows for screening of non-target compounds. TOF-MS can be used to discover "unknowns" post acquisition with no extra method development or cost, and with no reanalysis of the sample.