PW11 Routine Drug Screening by accurate mass using liquid chromatography/time-of-flight mass spectrometry and in source collision induced dissociation

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New API-Qq-TOF with ultra-high-resolution and ultra-high mass accuracy at high scan speed

Methods using liquid chromatography/time-of-flight mass spectrometry (LC/TOFMS) in the routine screening of drugs and their metabolites in equine urine samples have previously been described. These methods have been enhanced through the use of in-source CID (ISCID) to allow the detection of fragment ions in addition to the pseudo-molecular ions of target analytes. The incidence of false positive results is largely eliminated when the presence of such “qualifier” ions is used to distinguish analytes from near-mass interferences.
Databases were established containing the molecular formulas and the retention times of the compounds tested. Data processing software was used to create and integrate extracted ion chromatograms of the target pseudo-molecular ions in the database within a narrow mass window (±10mDa). The software evaluated the data by using matching criteria based on retention time, mass accuracy and isotopic pattern. Qualitative results were then reported automatically. This study required that the molecular formulae of each qualifier ion be determined in order to include its accurate mass in the database. Tentative identification of each fragment ion was made based on mass accuracy, isotopic pattern and chemical structure. Where possible these identifications were corroborated with the literature.
The methods described meet the required sensitivity for the large majority of the prohibited substances evaluated.