
Poster

[P27-7] P27-7: Assay

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[P27-7-3] Experience of using LC HRMS in full scan and PRM mode for reliable multi component urine drug screening

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Background

Immunochemical screening is still widely used in clinical and forensic laboratories for testing drugs of abuse in urine but may not longer cover sufficient number of analytes required to be analyzed in modern laboratories. Mass spectrometric methods may become a better alternative in terms of analysis efficiency, accuracy and reliability. The present work was aimed to design, validate and apply a multi-component LC-High Resolution (HRMS) method suitable for screening of a large number of new psychoactive substances, plant alkaloids and therapeutic drugs, in total 147 analytes, using an LC-Q-Exactive mass spectrometer (Thermo Scientific Co.)

Methods

The method consisted of dilution of urine (1:5) with 9 deuterated internal standards. The chromatographic system used a C-18 column and gradient elution with a flow rate of 0.5 mL/min. As solvents A and B were used ammonium formate buffer and methanol. The HRMS operated in ES positive mode with 70 000 resolution. The scan range was 100-650 amu and data for extracted ion chromatograms used ± 10 ppm tolerance. HRMS/MS was additionally applied in the same method for some selected analytes screening.

Results

Method validation demonstrated limited influence from urine matrix, linear response within the measuring range (for fentanyl 0.5 –1000 ng/mL and for the others 50 –1000 ng/mL) and acceptable imprecision in quantification (CV <15%). The reporting limit was set to 0.5 ng/mL for fentanyl and 1000 ng/mL for the others. Some analytes were found not to be stable in urine upon storage. The method was successfully applied in routine drug testing for analyses of 17936 unknowns. A total of 2715 (15%) positive samples were found to contain 52 of the 147 analytes investigated. QC results showed that the method was robust in routine work.

Conclusions

The method design based on simple dilution of urine and using LC-HRMS in XIC mode may offer an analytical system for urine drug testing that fulfils the requirement of automated, reliable and efficient solution that can replace immunochemical analyzers. It was important to apply a defined concentration reporting limit.