Poster

[P26-10] P26-10: Assay of toxicants

Chair: Steven How-Yan Wong, USA

Tue. Sep 26, 2017 12:30 PM - 1:30 PM Annex Hall (1F)

(Tue. Sep 26, 2017 12:30 PM - 1:30 PM Annex Hall)

[P26-10-1] Paper spray ionization for comprehensive drug screening - Are there chances to win a competition with established procedures?

Julian A. Michely[1], Markus R. Meyer[2], Hans H. Maurer[3] (1.Saarland University, 2.Saarland University, 3.Saarland University)

Keywords: paper spray ionization, HR-MS/MS, screening approach, drug testing

Background

Approaches for urine drug screening usually require sample preparation and chromatographic separation before detection by mass spectrometry (MS). Paper spray ionization (PSI) coupled to (high resolution, HR) MS might overcome these steps. So far, only target screening using PSI were described. The aim of this study was to develop a PSI-HR-MS/MS approach for comprehensive urine screening.

Methods

A volume of 20 L urine or neat sample was spotted onto Velox Sample Cartridges (Prosolia Inc., Indianapolis, USA) and dried at room temperature. Afterwards, the cartridges were directly analyzed using a Velox 360 paper spray autosampler with acetonitrile:water:formic acid (90:10:0.1) for eluting and transferring the compounds into a ThermoFisher (TF, San Jose, USA) Q-Exactive Focus HR-MS/MS system running in full-scan mode with data-dependent acquisition. For determination of influence by matrix or co-eluting compounds on analyte ionization, blank urine or water was fortified with 27 drugs (e.g. psychotropics, sedative-hypnotics, opioids, analgesics, stimulants, cardiovascular drugs) and glucuronides at 1 mg/L. Limits of identification were tested between 10,000 and 1 ng/mL. Finally, applicability was tested with authentic urine samples and proficiency test samples using automated data processing (TF TraceFinder 4.1) and a metabolite-based library (Maurer/Meyer/Helfer/Weber Library, Wiley-VCH, 2017).

Results

Matrix effects were between -23 and -100% whereby glucuronides particularly showed high ion suppression. Conjugate cleavage might overcome this disadvantage but would be an additional sample preparation step. Ion suppression/enhancement of co-eluting compounds ranged from +45 to -19% compared to single compound analyses. The limits of identification ranged from 10,000 to 20 ng/mL being in same range as for urinalysis after precipitation (Helfer et al., JCB, 2016).

Conclusions

The developed PSI-HR-MS/MS approach showed high matrix effects in urine because of missing analyte separation. Nevertheless, the identification limits for most compounds showed values comparable with established methods. Thus, PSI-HR-MS/MS might become a fast alternative for comprehensive screening but co-elution of analytes and endogenous compounds might be challenging for some drugs. For this purpose, further studies should be performed to estimate the extent and to overcome these limitations.