A novel method for automated detection and identification of toxicological relevant compounds in urine and serum samples using a GC/MS/NPD system

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INTRODUCTION: It is always very difficult and time consuming to identify a large number of target compounds in a high matrix background. The matrix may affect the ion ratios of target compounds, but typical target compound analysis requires finding the target ion and meeting the ratios of the qualifier ions. Therefore several manual steps like background subtraction; repeated library searches and manual integration are often practiced to solve the problem. This can take even for an experienced analyst more than one hour to review and confirm all compounds in a dirty matrix sample such as urine or serum extracts.

METHODS AND INSTRUMENTATION: Together with a quadrupole GC/MS system, a Nitrogen/Phosphorous Detector (NPD) and a combination of different powerful GC/MS techniques to create a fast quantification and screening tool was established to minimize additional laborious manual work following the analysis. Key of this method is the Deconvolution Reporting Software (DRS), which combines three different software packages: 1) standard GC/MS quantification software and databases, 2) the National Institute of Standards and Technology (NIST) Mass Spectral Search Program with the NIST05 MS library, 3) Automated Mass Spectral Deconvolution and Identification Software (AMDIS), also from NIST.

PRELIMINARY DATA: Different studies have been performed comparing conventional manual re-analyses and the automated DRS software. The automated quantification and screening tool reduced the data review process from hours of tedious work to minutes of unattended analysis. In many cases, the DRS software also eliminated false positive or negative results that have been found using traditional data analysis methods. An universal fast GC/MS method for the daily routine work on Forensic Toxicology samples on a 15m DB-17MS column together with a Retention Time Locked (RTL) forensic toxicology database developed by National Medical Services in Pennsylvania, USA as the target compound database was adapted for this evaluation. To broaden the range of drugs, which are accessible by GC/MS analysis, some entries in the databases of the used method are acetyl (CH_3CO), butyryl ($CH_3CH_2CH_2CO$) or pentafluoropropionyl (CF_3CF_2CO) derivatives.

CONCLUSION: This combination of techniques offers a fast, comprehensive, accurate, and least tedious method for screening and quantification of toxicological relevant compounds in high matrix samples.

KEYWORDS: *Mass Spectrometry, Gas Chromatography, µ-Fluidics-Splitter, Screening, Deconvolution, Databases, Complex Matrices*

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