**Introduction**

Liquid chromatography-mass spectrometry has become a valuable tool for qualitative and quantitative analysis of biological specimen in clinical and forensic toxicology. Meanwhile, many different approaches using various types of instruments and platforms are used to develop an ultimate comprehensive screening method to detect and definitively identify as many compounds as possible in a single run. Nevertheless, in daily routine work, the question for the detection of a dedicated set of substances e.g. hypnotics in cases of DFSA, psychotropics or benzodiazepines in DUJD cases arise quite often. Additionally, robust methods and hardware as well as easy-to-use software solutions gain more importance when analysing routine samples on a large scale. The aim of this project was to develop a spectral library of psychotropic drugs based on an open toxicology library concept recently developed with a comprehensive LC-MS\(^*\) screening approach (Toxtyper\(^{TM}\) Bruker Daltonik).

**Experimental**

The new library was used to assemble a scheduled precursor list (SPL) of 105 compounds to trigger data dependent acquisition of spectra. For method evaluation, different drug-free human serum samples and blank serum fortified with different mixtures of psychotropics, compiled according to the lower therapeutic concentration (\(c_{\text{LOW}}\)), were analysed. An ESI- and an ionBooster\(^{TM}\) source (IB), respectively, were used for ionization. In addition, all samples were analysed using the Toxtyper (TT) approach.

**Results**

In blank serum samples and samples fortified with two internal standards no compounds were identified and listed in the automatically generated reports. Two sets (\(c_{\text{LOW}}\) and 2x \(c_{\text{LOW}}\)) of 12 different mixtures containing a total of 96 compounds were analysed to evaluate the LODs for the automatic identification in serum. Using this screening approach and the ionBooster, 97 % of the analytes could be identified correctly at their respective \(c_{\text{LOW}}\). The Toxtyper screening detected 91 % of the included analytes at their \(c_{\text{LOW}}\).

**Conclusion**

The open library concept of the Toxtyper enables fast and easy generation of new qualitative methods for the detection of xenobiotics in human specimens. The method generated in this project is a fast and robust tool for the detection and identification of 105 medical psychotropic drugs in serum. Evaluation in spiked human serum samples showed detection of low therapeutic levels for the majority of compounds, making the screening applicable for clinical and forensic samples (intoxication and post mortem cases). The restricted number of analytes enables a more dedicated sample preparation and potentially allows upgrading the method to a semi-quantitative approach after additional LC optimization. The presented workflow can be transferred to other compound classes or subsets of analytes combined according to specific requirements in the lab.

**References**
