Liquid chromatography-mass spectrometry has become a valuable tool for qualitative and quantitative analysis of biological specimens 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 definitely 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 DFS, psychotherapeutics or benzodiazepines in DUII cases arise quite often. Additionally, robust methods and hardware as well as easy-to-use software solutions gain more importance when analyzing routine samples on an large scale. The aim of this project was to develop a spectral library of psychotropic medical drugs based on an open toxicology library concept recently developed with a comprehensive LC-MS<sup>3</sup> screening approach (Toxtyper<sup>™</sup> Bruker Daltonik).

**Introduction**

The open library concept of the Toxtyper<sup>™</sup> enables fast and easy generation of new qualitative methods for the detection of compounds of forensic interest (PS<sub>4</sub>). Using this approach and the ionBooster, 97 % of the analytes could be identified correctly at their respective concentration. The Toxtyper screening detected 91 % of the included analytes at their LOQ. Perphenazine and thioproperazine were both not detected at the LOQ = 1 ng/ml. Perphenazine showed the least analytical enhancement (factor 3) when using the ionBooster, while thioproperazine revealed undesirable chromatographic behaviour under the rather generic LC conditions used. The higher number of precursor masses in the SPL of the Toxtyper screening might explain the lower percentage of correct findings at low concentrations.

**Results**

The results from our routine analysis of serum samples (QqQ) of several cases with known intake of psychotropic medical drugs were confirmed with positive findings, if the concentration range was above or around the assumed limit of detection from this evaluation study. Even in highly complex matrices like post mortem serum, analytes could be detected and identified correctly at sub-therapeutic levels along with toxic concentrations of other compounds as shown in samples #3 and #4.

**Conclusion**

The open library concept of the Toxtyper<sup>™</sup> 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 psychotropic medical 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 specimens (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**


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