

Toxicological Screening and Quantitation Using Liquid Chromatography/Time-of-Flight Mass Spectrometry

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In recent years, an increasing number of new designer-drugs have increased the demands for general toxicological screening [1]. Limited screening based on immunoassays is commonly used in clinical toxicology, whereas more comprehensive approaches are common in forensic toxicology such as screening based on Gas or Liquid Chromatography (GC or LC) approaches [2]. The classic approach has been gas chromatography-Mass Spectrometry (GC-MS) combined with LC-diode-array detection (DAD) for systematic toxicological analysis. This setup has the advantage of covering a very broad spectrum of drugs and illicit substances when combined with library search facilities. However, the analytical sensitivity and specificity of LC-DAD may not be optimal. Thus, more sensitive and specific screening techniques based exclusively on LC combined with mass spectrometry have gained popularity. Multi-target screening and quantitation methods based on LC-tandem mass spectrometry (MS/MS) may provide detection of hundred or more compounds [3]. Using ion-trap MSn detection, several hundred compounds can be detected [4]. A more extended screening is possible using time-of-flight (TOF) mass spectrometry, which is a high-resolution mass spectrometry technique that detects drugs on the basis of their exact mass. Using this technique, scanning is performed over all masses for low molecular drugs, and detected signals can be related to a library of exact drug masses. Retention time and fragmentation pattern contribute to the identification. In principle, it is possible to screen for thousands of compounds, although issues related to software capabilities may limit the number of compounds to several hundred in daily practice [5-7].

Having detected compounds in toxicology, quantitation is usually also desired. Several techniques are available, e.g. GC, LC-DAD, GC-MS and LC-MS/MS. LC-MS/MS is generally regarded as the optimal approach, having unsurpassed sensitivity, specificity and dynamic range [3]. However, LC-TOF-MS may not only be used for screening but also for quantitation as recently investigated by several authors [8-10]. The dynamic range and sensitivity may not match those of LC-MS/MS, but may still be acceptable. Liquid

chromatography-mass spectrometry equipment is generally expensive, so a combination of screening and quantitation by the same equipment is both practical and of advantage from an economical point of view, in the paper by Dalsgaard, et al. [11], in this issue of the journal, quantitation of common drugs of abuse in blood by LC-TOF-MS is considered.

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