

## Simultaneous analysis of drugs in forensic cases by liquid chromatography–high-resolution orbitrap mass spectrometry

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### ABSTRACT

In the present study, liquid chromatography coupled to an Orbitrap mass spectrometer (HPLC–Q-Orbitrap MS) was used as an approach for identification and quantification of 113 drugs simultaneously in biological samples (whole blood/plasma/serum). Samples were prepared using liquid–liquid extraction conducted using a trizma/isopropanol/butyl chloride buffer system. Reversed-phase separation employing a column (50 × 2.1 mm) packed with 2.6- $\mu\text{m}$  C18 particles was then performed under gradient elution with mobile phase composition consisting of acetic acid and aqueous-acetonitrile mixtures with the acetonitrile content ranging from 10 to 100% v/v. Compounds were detected with high-resolution MS operated in full scan mode having a mass accuracy < 5 ppm. In this study, isobaric compounds (same nominal mass) were easily distinguished and identified by their different retention times. Extracted ion chromatograms (XICs) with narrow mass tolerance window (5 ppm) provided analysis with acceptable linearity ( $r^2$ ) ranged from 0.9530 to 1, low limits of detection (LOD) (0.02–39 ng mL<sup>-1</sup>) and low limit of quantification (LOQ) (0.1–130 ng mL<sup>-1</sup>). The developed method was applied to successfully analyse drugs in 26 blood samples from positive forensic cases and proved that this technique was able to detect analytes at trace level.

### KEYWORDS

Blood analysis; Drug screening; High-resolution mass spectrometry; Liquid–liquid phase extraction; UHPLC–HRMS

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