

der the application of Nd<sup>+</sup> ion technique. Recently, we initially developed a new analytical method by thermal ionization mass spectrometry (TIMS) for precise <sup>143</sup>Nd/<sup>144</sup>Nd ratio analysis as Nd<sup>+</sup> ions with film porous ion emitters (FPIEs), combined with a simplified Nd chemical separation procedure. The Nd<sup>+</sup> ion yields of the method were one order of magnitude higher than that of traditional Nd<sup>+</sup> ion analysis method, and is even comparable with those of NdO<sup>+</sup> ion analysis method reported previously. The possible mechanisms of FPIEs in improving sample utilization and reproducibility of Nd isotope ratio analysis were discussed as well. Repeated measurements of 1 ng reference material JNdi-1 yielded a <sup>143</sup>Nd/<sup>144</sup>Nd value of 0.512113 ± 33 (2SD, n=9). The achieved external precisions fulfilled the requirements for applications in nuclear forensics. Several international rock reference materials with a wide range of matrix composition and uranium ore samples were also analyzed to further verify the accuracy and reproducibility of our method. The newly-developed TIMS approach is much less laborious and time-consuming, and we believe that this method is not merely of particular value for nuclear forensic purposes, but also expands the applications in geochemistry, geochronology and environmental sciences.

**Keywords:** Neodymium isotope, Thermal ionization mass spectrometry, Nuclear forensics

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## Development and validation of a bioanalytical assay to detect biomarkers for antidepressant use in influent wastewater

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Wastewater-based epidemiology applies the analysis of human metabolic excretion products of xenobiotics in wastewater to estimate the community-wide use of these compounds. The low ng/L range of concentrations of biomarkers present in a complex matrix such as wastewater pose a clear bioanalytical challenge related to sample preparation and detection/quantification. Therefore, sensitive bioanalytical methods need to be developed, optimised and validated for the detection and analysis of a broad range of selected biomarkers at trace concentrations in influent wastewater.

We developed and validated an analytical approach based on solid-phase extraction and liquid chromatography coupled to tandem mass spectrometry for the simultaneous detection and quantification of 27 antidepressants and their metabolites in influent wastewater. For most compounds, Oasis<sup>®</sup> HLB cartridges were used for sample preparation. Oasis<sup>®</sup> MCX cartridges were used for extraction of normirtazapine, moclobemide, sertraline, and melitracen in particular. The Kinetex XBC18 column with a gradient elution resulted in appropriate separation for the analytes under investigation. Validation was done according to the European Medicines Agency guidelines on bioanalytical method validation and the performance criteria met the requirements. For these analytes, the lower limit of quantification (LLOQ) ranged between 1 and 25 ng/L. Furthermore, all targeted biomarkers showed high in-sample stability during 24 h, with the exception of mianserin. In addition, all compounds under investigation showed high on cartridge-stability (< 20% transformation) after 1.5 months of storage at -20 °C in an air-tight freezer bag. For five compounds, the deuterated analogue used as internal standard (IS) did not correct for matrix effects and highlights the need of a thorough assessment of matrix effects during method validation even if deuterated analogues are used as IS. The validated assay was applied to influent wastewater samples collected from four wastewater treatment plants in Belgium. Among these four locations, a total of 18 out of 27 biomarkers for antidepressant use were present in the samples in concentrations above the LLOQ. The results could be used to look at spatial and temporal trends in antidepressant use.

**Keywords:** Method development and validation, wastewater analysis, antidepressants

Graphical Abstract



This file includes the graphical abstract.