

HARMONISED APPROACH OF NON-TARGET SCREENING FOR EMERGING CONTAMINANTS IN HUMAN URINE BY LC-HRMS

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Background: Contaminants of emerging concern (CECs) are not included in monitoring programs because the lack of data. Non-target screening analysis of human urine samples by high resolution mass-spectrometry (HRMS) can provide an overview of the presence of CECs in the population. However, there is a lack of harmonised methods that permit obtaining comparable and high-quality results. To facilitate the development of reliable and comparable non-target/suspect screening workflows for the assessment of CECs in human urine by LC-HRMS, we have developed a generic quality assurance (QA)/ quality control (QC) framework.

Methods: The achievement of an actual and representative fingerprint of CECs in human urine is a challenge that requires the establishment of proper QA/QC measures for each individual step considering their impact in both individual steps and the global workflow. The developed non-target screening method was applied to the analysis of human urine for the quantification of CECs. A well-structured algorithm based on the Schymanski-scale to enhance and simplify the data processing has been developed and submitted to benchmarking studies.

Results: Crucial QA/QC measures have been implemented in the analytical workflow, such as the addition to the urine samples of a set of labeled standards in a wide range of chemical properties or running in parallel procedural blanks. The results of benchmarking experiments proved the capability of the developed workflow to obtain comparable and high-quality results. The analysis of urine samples resulted in information over the detection frequency of CECs.

Short discussion/conclusions: Although the CECs present in human urine are (yet) unknown, a good point to evaluate the whole non-target/suspect screening workflow may be the comparison with the obtained results by applying available well-defined target approaches to the same urine samples. Anyway, more effort in this direction is still needed owing to the premature status of the major workflows in this field.