Strategies for Suspect and Non-target Screening of New Emerging Chemicals in Human Biomonitoring

GC/LC-HRMS Measurement Techniques of Human Matrices and Data Mining of Mass Spectrometry Data for High Throughput Analysis

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Introduction

Humans are exposed to a large number of chemicals from consumer products, foods, and through environmental media. To assess this exposure, human biomonitoring (HBM) analyzes chemicals in human fluids and tissues. Typically, only a small number of chemicals are covered in targeted methods.

Non-target screening (NTS): Screening in full scan mass chromatograms for a list of molecular structures of compounds expected in the sample without using a reference standard, with a subsequent tentative identification of suspect hits.

Non-target screening (NTS) - Structures of compounds expected in the sample without using a reference standard, with a subsequent tentative identification using mass spectrometric information and eventually meta information. For both strategies, final unambiguous identification of masses is done by comparison to reference standards (targeted analysis).

Main Objectives

The overall aim of this PhD project is the development of suspect and non-targeted screening methods for the detection of a wide range of suspects in human matrices based on liquid and gas chromatography coupled to high resolution mass spectrometry (GC- or LC-HRMS) and to apply these methods for the assessment of human exposure in cohorts studies within the work package 16 of the project Human Biomonitoring for Europe HBM4EU (www.hbm4eu.eu). Current projects:

1. Suspect screening methodology on a predefined list of emerging contaminants (xenobiotic amines) on a sample set of a human matrix (urine) using state of the art open source high performance computational tools for prediction and verification.

2. Method development of a non-targeted workflow to compare in vitro formed metabolites of pesticides with the occurrence in human samples.

Challenges and Limitations

- Xenobiotic compounds are typically small peaks against the biological background.
- The substance of interest is typically metabolised resulting in a number of phase I and phase II metabolites.
- While targeted methods rely on the availability of a reference standard, screening techniques rely on prediction techniques to narrow down the list of tentative candidates.
- Screening techniques cannot provide quantitative results but can deliver qualitative results. This results in a list of possible biomarkers of exposure for further targeted analysis.
- HBM relies on large sample sets to account for individual variation. This results in large datasets for subsequent processing.

Acknowledgements

This project has received funding from the European Unions Horizon 2020 research and innovation programme under grant agreement No 733032—HBM4EU.