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# Widening exposome exploration by means of complementary HRMS analytical platforms: use case on pesticide exposure

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## Introduction

Human exposure to food and environmental contaminants (such as pesticides) is generally estimated by indirect methods.

Targeted bio-monitoring is a way to assess the internal exposure on a limited number of substances, needing large sample amounts for analyses as rigorous and sensitive as possible. Thus, the human health risks associated with multi-exposure to complex mixtures currently remain under-explored.

In this context, the SCREENPEST project aims at providing a unified methodology for large-scale characterisation of human internal exposure to pesticides, via a "suspect profiling" approach, using urine.



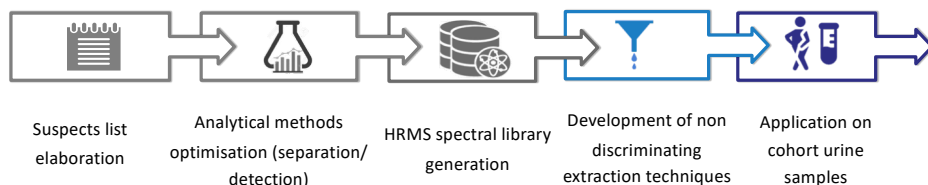
## Objectives

Develop and set-up an harmonised analytical workflow including sample preparation, instrumental measurement and data processing. Increase the coverage on human exposure to pesticides by a non-targeted multiplexed approach.

Test the method developed through urine samples from cohorts to study possible links between exposure and adverse health effects.

Provide extended information capabilities for early warning on emerging substances and help for decision making.

## Developed workflow



### PÉLAGIE

- Mother-child cohort (France, 2002-2006)
- Association between the exposure to pesticides of pregnant women and biometric data at birth
- Access to 168 samples



### NutriNet-Santé

- General population (France, since 2009)
- Association between the exposure to pesticides and the onset of type 2 diabetes
- Access to 200 samples

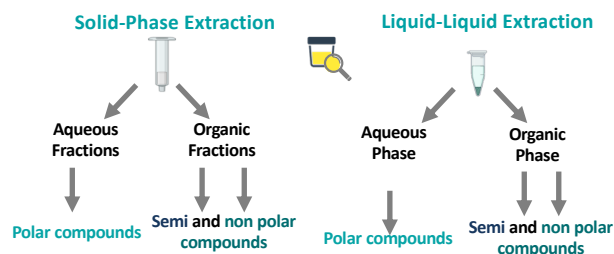
## Method development

**Large list of standards** (ca. 200 pesticides and phase I/II metabolites), covering a wide range of physicochemical properties (logKow: [-4.71;8.38], MM/g.mol<sup>-1</sup>: [72;720]) for analytical developments. Standard selection: commercial availability, bibliography, pesticide use in France (2019), epidemiologists expertise and available data from the HMB4EU project (10.1021/acs.analchem.2c00061)

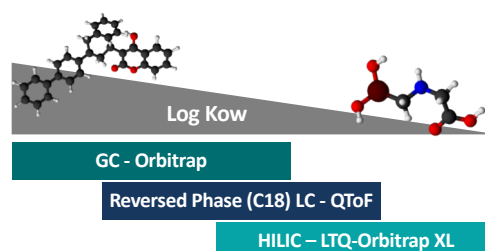
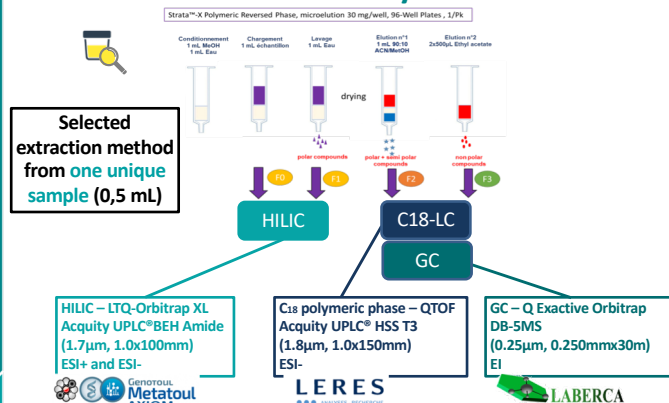
**Optimisation of 3 HRMS techniques** to get the best separation and detection of the suspects by both LC and GC. Characterisation of the suspects by HRMS

**Optimisation of sample preparation:** various concentration levels (20, 50 and 100 ng mL<sup>-1</sup>) spiked in pooled urine (5 replicates).

Performance comparison of two non discriminating extraction techniques (recovery and matrix effect)



## Extraction and HRMS analysis



Analytical challenges to cover a wide range of compounds with:

- Different physicochemical properties :
  - Mol. weight [72;720]
  - Polarity / Log Kow [-4.71;8.38]
- Poorly characterised biotransformation products
- Low levels concentration

## Data treatment - Bioinformatic tools

Extended HRMS spectral library of reference pesticides and metabolites.

Complemented in house non-targeted and suspect screening chemo-informatics tools (XenoScreener / PeakForest / MetaboHUB W4M).

Improved annotation and identification capacities on a large range of pesticides

Statistical analysis and data interpretation (in progress)