The challenge to produce robust data in UHPLC-HRMS/MS based metabolomics for molecular epidemiology studies
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To cite this version:
Quentin Vandoolaeghe, Claire Lopez-Piffet, Valérie Bouchart, Raphaël Delépée. The challenge to produce robust data in UHPLC-HRMS/MS based metabolomics for molecular epidemiology studies. Congrès ANALYTICS 2022, Sep 2022, Nantes, France. hal-03846429

HAL Id: hal-03846429
https://normandie-univ.hal.science/hal-03846429
Submitted on 10 Nov 2022
Context: Agricultural activity and cancer

Link between occupational exposures and cancers demonstrated in farmers

- Study cancer biological plausibility, early stages effects, lookout for predictives markers of cancer risks
- Holistic approach of cancers occurrence in farmers population

Utilisation of biobanks samples associated with exposure description and tasks listing for a metabolomic analysis

Potential available matrix

- Blood
- Urine
- Saliva
- Hair

Metabolomic

General Workflow

1. Experimentation design
2. Sample preparation
3. Metabolites separation
4. Ionisation
5. Detection

Many steps to be optimized

No general method for metabolomic analysis of human urine samples in the literature

Setting up of a test study on healthy volunteers

Men urine samples

Women urine samples

Results

5 mobile phases comparison

Signal normalisation comparison

- Osmolarity
- Creatinine
- Total MS signal

Groups separation and markers highlighted

Methodology

Chromatographic parameters and HRMS detection

- Separation of low polarity molecules
  - C18 Waters Acquity® BEH C18 (1x100mm; 1,7 µm)
  - ESI Positif
  - ESI Negatif

- Separation of high polarity molecules
  - HILIC Waters Acquity® BEH amide (1x100mm; 1,7 µm)
  - ESI Positif
  - ESI Negatif

Masse detection: QTOF Agilent 6540, 1 scan/sec, 50-1000 m/z

Data treatment: Galaxy W4M & mixOmics

Perspectives

- Ion annotation tool optimisation
- Biobank samples analysis
- Study on blood, hair or saliva
- Use of new statistical tools