DEVELOPMENT OF A DATA PROCESSING WORKFLOW FOR NON-TARGETED METABOLOMICS ANALYSIS USING GC×GC-TOFMS

Pierre-Hugues Stefanuto[1] ; Delphine Zanella[1] ; Lena M. Dubois[1]; Jean-François Focant[1]

[1] Organic and Biological Analytical Chemistry Group, MolSys, University of Liège, Belgium

Abstract

The constant improvement of analytical instrumentation generates more and more insights for non-targeted metabolomics. In this context of untargeted screening of complex biological mixtures, comprehensive two-dimensional gas chromatography (GC×GC) coupled to time-of-flight mass spectrometry (TOFMS) offers a powerful solution to obtain a detailed overview of sample compositions. However, the increase of analytical resolution comes with an increase of system and data complexity [1,2]. This generates a critical need for clearly defined adequate method optimization and quality control (QC) protocols to insure the proper use of the analytical instrument. Extremely important is also a robust data processing flow for interpretation. Unfortunately, few untargeted GC×GC studies display these important aspects and a general misuse of the terms validation and semi-quantification are flourishing in the related literature. These bias are contributing to the general problem of lack of study reproducibility in some aspects of scientific research, as pointed out in recent Nature publications [3,4]. To overcome this problem, several initiatives such as the metabolomics standard initiative (MSI), set up some general guidelines to reduce such lack of analytical robustness [5,6].

One of the major working area is the definition of a clear reporting method for the data processing workflow to insure unbiased statistical treatment, and allow any scientist to reproduce it. In the context of publicly available data, the transparency of the data processing is crucial. This study proposed a defined way to present the processing workflow from GC×GC-TOFMS output. It is based on examples coming from different metabolomics applications.

References

[1] P.H. Stefanuto et al. Anal. Bioanal. Chem. 407 (2015) 4767–4778.
[2] P.H. Stefanuto et al. J. Chromatogr. A. 1507 (2017) 45–52.
[3] M. Baker Nature. 537 (2016) 703–704.
[4] M. Baker Nature. 259 (2016) 456–458.
[5] L.W. Sumner et al. Metabolomics. 3 (2007) 211–221.
[6] R. Goodacre et al. Metabolomics. 3 (2007) 231–241.