Development of data processing workflow for untargeted multidimensional chromatography

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During the last decade, comprehensive two-dimensional gas chromatography coupled to mass spectrometry (GC×GC-MS) has become a mature technique. The constant improvement of the hardware (e.g., high speed MS, modulators) and controlling software have generated robust commercial systems. GC×GC-MS has now entered a new phase of extended applications in different fields. Indeed, GC×GC-MS is now commonly used to conduct large scale studies, giving full access to its high-resolution power for targeted and mostly untargeted screening. This high-resolution in the separation is particularly helpful for complex samples untargeted screening, as commonly encountered in metabolomics. The current challenges of the technique are now localized on the data management side, where powerful chemometric tools are required to unlock GC×GC-MS full potential.

In order to tackle those challenges, we have been investigating specific chemometric tools for GC×GC-MS in the aim of developing user friendly data processing solutions. An optimized processing workflow is a key to ensure data quality. To understand the impact of each data processing step, each of the critical steps of data preprocessing, feature selection, model building, and validation have been investigated in detail using different data sets.

From this investigation, we have designed a guide for users who desire to establish robust and reproducible GC×GC-MS data processing workflows. This guide also evaluates the user impact in the data processing and how it can bias the data. We have also investigated the development of the next generation of chemometric tools, looking to artificial intelligence and machine learning.

Reference:

PH Stefanuto, A Smolinska, JF Focant, Advanced chemometric and data handling tools for GC×GC-TOF-MS: Application of chemometrics and related advanced data handling in chemical separations, TrAC Trends in Analytical Chemistry, Volume 139, 2021.