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## CONTRIBUTION OF GC×GC-(HR)-TOFMS TO MEDICAL APPLICATIONS

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Comprehensive two-dimensional gas chromatography (GC×GC), especially when coupled to time-of-flight mass spectrometry (TOFMS), has come a long way since the original report on the technique [1]. Several robust modulation devices (cryogenic modulators, flow modulators, solid state modulators, …) are now available and cover most fields of applications. Current GC×GC-TOFMS instruments allow to separate thousands of signals for semi-routine analyses of large sets of samples. Data processing however still remains the bottle neck of the technique and requires complex dedicated procedures to properly extract the relevant information from the tremendous quantity of multidimensional data, especially when high resolution (HR)TOFMS is used.

Amongst the numerous fields of application of GC×GC-TOFMS, medical applications are of high interest as they ultimately can play a role in public health at a large scale. Such applications include search for biomarkers of illness and understanding of metabolic processes. These type of studies usually require profiling volatile organic compounds (VOCs) present in breath; measuring headspace VOC signatures from blood, urine, feces, and cultured cell media; or performing metabolite screening on plasma samples…

For each of these, it is important to develop and optimize proper sampling procedures often based on solid-phase microextraction (SPME) or thermal desorption (TD). The implementation of robust chromatographic methods is also crucial to ensure that high quality signals are produced prior to any data processing. Then, the most important aspects to be considered are data alignment, data reduction, (un)supervised statistics, and visualization of results. Several data mining approaches and statistical tools (Fisher ratio, PCA, PLS, clustering, machine learning…) have been implemented to digest the large amount of data generated. This will be illustrated through recent achievements in the medical field.

Reference

[1] Liu Z. and Phillips J.B., J. Chromatogr. Sci. 29 (1991) 227–231.