

GC×GC-TOFMS for Medical Volatolomics

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When speaking about cutting-edge advances in GC, the introduction of high peak capacity comprehensive two-dimensional gas chromatography (GC×GC) is probably the bigger move since capillary columns appeared. Both cryogenic zone compression signal enhancement and chemical-dependent structuration of elution patterns make the uniqueness of the technology. When hyphenated to (high resolution) time-of-flight mass spectrometry ((HR)-TOFMS) and the related mass spectral deconvolution efficiency, it provides one of the most powerful tools in separation sciences today.

Over the last few decades, medical volatolomics has been keeping constant attention of the medical community as measuring volatile organic compounds (VOCs) related to human specimen has often been reported as one of the most promising low invasiveness approaches for potential diagnosis of various diseases. Indeed, the fingerprint of VOCs present in the exhaled air or in the headspace/liquid part of various biofluids of a patient are linked to metabolic pathways taking place in the body and are impacted by pathologies, especially in the case of pulmonary diseases, but not only as VOCs are blood-borne chemicals.

Over the last few years, we tested various matrices and sampling approaches for GC×GC-(HR)-TOFMS to isolate putative biomarkers or chemical profiles to build diagnostic models following strict QA/QC protocols. Advanced chemometric and data handling tools were studied to obtain complete data processing workflows including in-depth validation of the statistical models used. This was applied for multicentric breathomics of different lung diseases such as for asthma phenotyping, as well as for detecting metabolomic alterations associated with systemic sclerosis (SSc) and its pulmonary complication known as interstitial lung disease (ILD). A multi-derivatization-based metabolomics/lipidomics profiling method of blood from colorectal cancer (CRC) patients at various stages of the disease was also successfully developed.