GC(xGC)-13

Tackling challenges for the adoption of two-dimensional gas chromatography in Forensic Sciences

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In the last decade, comprehensive two-dimensional (2D) gas chromatography (GC×GC) has been successfully established as an essential tool for the analysis of complex mixtures in the field of environmental science, in the petrochemical industry, and for the exploration of biological samples. Despite its numerous advantages in comparison to one-dimensional (1D) GC, such as increased peak capacity, higher sensitivity and the possibility of group-type analysis, its application in forensic sciences remains rather limited. A major reason is that the adoption of a novel analytical technique to the needs of the modern forensic science laboratory is usually lengthy and challenging due to the strict requirements that are enforced in forensic laboratories. The time investment for method validation through laboratory accreditation, as well as potentially increased acquisition and maintenance costs, are both contributing factors to reluctance in the field. Regarding the implementation of GC×GC-based techniques, doubts may arise whether information could be lost using this new technique, because only few studies have been presented documenting method translation from 1D GC to 2D GC in forensic sciences to ensure that there is no loss of metadata. However, in the case of GC×GC, more information about sample composition is acquired in comparison to 1D GC. Therefore, additional software tools are needed to assist with the process of extracting meaning from multivariate data for objective decision-making. Furthermore, the complexity of the technique, a limited degree of automation in the workflow, and the need for additional training for laboratory technicians and scientists, are significant factors that impede full adoption in forensic laboratories.

Conventionally, novel GC×GC instruments were provided as a packaged solution. However, increasing options are becoming available to retrofit existing GC-MS systems, such as those available in forensic laboratories currently using traditional quadrupole MS (qMS). This may serve to make GC×GC more accessible to industries that are reluctant to purchase and adopt a completely new technique over their pre-existing instrumentation and workflows. Also, with the increasing improvements in quadrupole mass spectrometer scan rates, these tools now have increasing options for coupling to GC×GC. In this study, a GC×GC with qMS and simultaneous flame ionization detector (FID) with a reverse fill/flush (RFF) flow modulator was employed to exploit higher flows and slightly wider peaks in a dual detection approach. The objective of this study was to demonstrate quality assurance procedures when translating a GC-qMS method to a GC×GC-qMS/FID instrument using reverse fill/flush modulation retrofitting for the analysis of volatile organic compounds (VOCs). Figures of merit and calibration curves using GC-qMS and GC×GC-qMS/FID are presented, documenting the transfer and adaptation of the original method without a loss in data quality.