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FINGERPRINTING OF EXTRA VIRGIN OLIVE OIL VOLATILES BY GC×GC: METHOD TRANSLATION AND METADATA TRANSFER FROM THERMAL TO DIFFERENTIAL FLOW MODULATED PLATF

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Fingerprinting is an investigation strategy aiming at comprehensively mapping characteristic patterns of chemicals for effective cross-sample analysis. Comprehensive two-dimensional gas chromatography is a technique at the same time combining the advantages and the information power i) of a detailed sample profiling, by informing about the quali- and quantitative distribution of target chemicals, and ii)of producing unique bi-dimensional (2D) patterns (fingerprints) to be used for samples discrimination and classification. In this context, the possibility to perform routinely highly informative fingerprinting on large sample set is attractive but, nowadays, also requires a) analytical platforms connoted by low operational costs while avoiding the use of cryogenics, and b) simple laboratory operations with limited analyst supervision during intensive analytical sessions.

This study explores the feasibility of transferring a fingerprinting method for extra virgin olive oil volatiles from thermal modulated (TM) GC×GC-MS to a differential flow modulated (FM) platform implementing a reversed-fill-flush injection dynamics.

The principles of method translation are adopted to transfer effectively the application from TM-GC×GC to FM-GC×GC by preserving analytes elution order, 1D resolution, and 2D pattern coherence.

Different column combinations (length, internal diameter and film thickness) and configurations (dual parallel secondary columns or post-column splitting to MS/FID) are considered for effective translation and to match for analytical constraints posed by FM-GC×GC.

Experimental results confirm the feasibility of method translation, its effectiveness in preserving elution order and original method resolution, but highlight the need of a careful evaluation of the peculiar nature of FM-GC×GC. If not, the risks are that structured patterns of chemicals are lost, the number of detectable compounds reduced by half and/or the overall separation power of the translated method decreased of about 80%.

The configuration that performs better includes a narrow bore (i.e. 0.1 mm dc) column in the 1D and dual-parallel columns in the 2D. This set-up enables operation under close-to-optimal conditions in the 1D with the FM-GC×GC besides the lower overall method sensitivity due to the effluent splitting in two secondary columns. Nevertheless, fingerprinting accuracy and discrimination power are preserved.