Challenges and Opportunity: Translating advanced fingerprinting methods from thermal to differential flow modulated GC×GC

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Abstract

The possibility to transfer methods from thermal to differential-flow modulated comprehensive two-dimensional gas chromatographic (GC×GC) platforms opens interesting perspectives for routine analysis of complex samples. Flow modulated platforms avoid the use of cryogen, thereby simplifying laboratory operations and analyst supervision.

The study investigates the feasibility of transferring a fingerprinting method for volatiles capable of classifying and discriminating high-quality cocoa according to origin and processing. The principles of GC×GC method translation are applied to an original fingerprinting method, developed for a loop-type thermal modulated GC×GC-MS system, to create a method adapted to a reverse-injection differential flow modulated platform with a dual-parallel secondary column and dual detection (GC×2GC-MS/FID).

Effective method translation preserves analytes elution order, ^1D resolution, and ^2D pattern coherence. Results confirm the feasibility of translating fingerprinting method conditions while preserving the informative power of 2D peak patterns for sample classification and discrimination.

Correct translation enables effective transfer of metadata (e.g., compound names and MS fragmentation patterns) by automatic template transformation and matching from the original/reference method to its translated counterpart. Fingerprinting accuracy is preserved and most of the key-aroma compounds and technological markers are effectively mapped.

ISCC & GCxGC 2017