## POTENTIALS OF THE REVERSED-INJECT DIFFERENTIAL FLOW MODULATOR COMPREHENSIVE TWO-DIMENSIONAL GAS CHROMATOGRAPHY IN THE QUANTITATIVE PROFILING OF SUSPECTED FRAGRANCE ALLERGENS

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Multidimensional Gas Chromatography (MDGC) is a separation technique with great potentials in the (quantitative) profiling of very complex mixtures of volatiles [1] and, when implemented in "comprehensive" configurations (GC×GC), is capable of higher separation power, unmatched peak capacity and meaningful 2D elution patterns that facilitate analytes identification while providing distinctive sample's fingerprints.

Thermal modulators, and in particular those implementing a cryogenic device [2], are widely used for volatiles' profiling because of their very efficient band focusing that avoids break-through phenomena. However, these modulators have also some drawbacks mainly related to the high costs in term of hardware and operations limiting their adoption for routine quality controls and high-informative throughput screenings [3].

In this contribution the first Capillary Flow Technology (CFT) reverse-inject differential flow modulator is implemented with different column configurations (lengths, diameters and stationary phase coupling) and detector combinations (Mass Spectrometry - MS and Flame Ionization Detection - FID) to evaluate its potential in the quantitative profiling of suspected allergens in medium-to-highly complex fragrances.

System performance parameters (separation measure  $S_{GC\times GC}$ , Modulation Ratio  $M_R$ , separation space used and peak symmetry) have been evaluated on a model mixture including 62 chemicals listed in the Scientific Committee on Consumer Safety (SCCS) Opinion on fragrance allergens in cosmetic products (1459/11 -26/27 June, 2012). Within the different column combinations tested, the system demonstrating the best chromatographic performance has been selected for quantitative profiling of fragrance allergens.

The optimization tuning of column dimensions and system detection configuration (parallel MS/FID detection) enables to achieve: (a) very high 2D separation power, (b) highly reproducible 2D patterns, (c) synergic data treatment between FID and MS detection and, (d) effective handling of overloaded peaks without dramatic losses in resolution and quantitative accuracy.

## References

[1] PJ Marriott et al. Trends Anal Chem 34 (2012) 1-21

[2] PQ Tranchida et al. Trends Anal. Chem. 30 (2011) 1347-1461

[3] C Cordero et al. J. Chromatogr. A 1147 (2015) 79-95