GC×GC with parallel detection by FID and TOF MS featuring tandem ionization: extra-dimensions for great flexibility in fragrance allergens profiling

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Abstract

Comprehensive two-dimensional gas chromatography coupled to mass spectrometry demonstrated to be the technique of choice for quantitative profiling of complex samples of fragrance raw materials and perfumes [1,2]. High separation power and sensitivity achieved by band-compression in space obtained by thermal modulators enables confident characterization for regulated substances.

In this study, a GC×GC platform equipped with a loop-type thermal modulator, parallel detection by flame ionization detector (FID) and time of flight mass spectrometry featuring Tandem Ionization™ is adopted for detailed quali-quantitative profiling of the extended set of fragrance allergens [3]. Spectral dissimilarity between "hard" (70 eV) and "soft" ionization (12 and 14 eV) is measured through a standardized metrics (i.e, NIST Similarity search algorithm) while relative detection sensitivity is evaluated by comparing signal to noise ratio (SNR) values for representative analytes. The parallel detection by FID and TOF-MS is then examined for linearity performance within a range of concentrations of interest for fragrance raw material characterization. Dynamic range of response and linearity are also compared between single ionization and tandem ionization acquisition while the FID is validated for predicted relative response factor quantitation [4].

Results confirm that multi-parallel detection provides great flexibility enabling confident analytes quantitation in samples with highly-variable composition. In addition, low-ionization energy offers the possibility to exploit an additional spectral dimension improving method specificity and selectivity, especially when complex coelution issues occur.

References

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