Quantitative analysis of allergens in perfume samples using comprehensive two-dimensional GC (GCxGC) and Time-of-Flight Mass Spectrometry (TOFMS)

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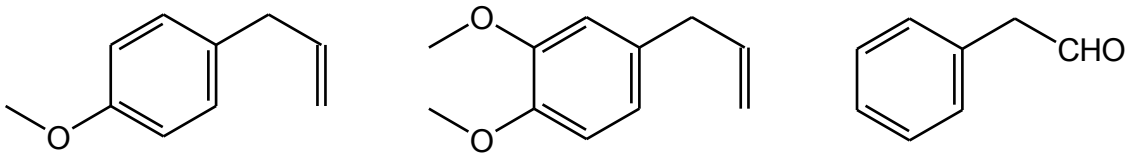
Fragrances are complex mixtures that are part of the everyday life. From cosmetics to household products, chemicals that produce scents are present at various levels, but little is known about their composition since fragrance formulas are considered trade secrets. New concerns about the health risk posed by some of their chemicals, either purely synthetic or of natural origin, have lead to an increased interest in the composition of fragrance. The 7th Amendment of the European Cosmetic Directive requires to declare the listed 26 "fragrances allergens" (24 defined volatile substances and 2 botanicals) if they exceed specified levels. As a result, a project was initiated at the end of 2001 within the International Fragrance Association (IFRA), to develop a method for the analysis of "fragrances allergens", with the purpose of defining a way to determine and regulate their presence (*1*) (*2*).

Comprehensive two-dimensional gas chromatography (GCxGC) provides the additional peak capacity necessary to solve the composition of complex sample mixtures. Two separation mechanisms are employed to aid in the analysis of such complex samples. With thermal modulation, peak widths at the end of the second column are typically in the order of 100 ms and fast data acquisition systems are required. Time-of-flight (TOF) MS is the only mass spectrometer capable of acquisition rates up to 500 spectra/s, adequate for the characterization of peaks as narrow as 20 ms.

This study is concerned with the detection in perfumes of 24 above-cited targeted compounds and 3 additional volatile items (namely: estragole **1**, methyleugenol **2** and phenylacetaldehyde **3**), concerned by other regulatory issues.



1 2 3

A GCxGC-TOFMS system is used to find, identify and quantitate the presence of all components in one analysis. A comparison between a one-dimensional and a two-dimensional analysis as well as a comparison between different column combinations will be presented.

References.

(*1*) A. Chaintreau, *Analysis of allergens in fragrances : an analytical challenge*. Paper presented at the 35th International Symposium of Essential Oils, Messina, Italy, 29 Sept.-2 Oct. 2004.
(*2*) A. Chaintreau, D. Joulain, C. Marin, C.-O. Schmidt and M. Vey. *GC-MS quantitation of fragrance compounds suspected to cause skin reactions. 1.* J. Agric. Food Chem. 2003, **51**, 6398-6403.