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JSB-DP004

GC×GC-MS analysis of aroma compounds and allergens in perfumes

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Introduction

Perfumes are complex mixtures that can consists of hundreds of natural and synthetic compounds. They often include numerous fragrance-key components present in low amounts. Chemical profiling is therefore challenging. On the other hand, accurate speciation is of key importance for quality control as well as for monitoring allergens subjected to regulations. GC-MS is the natural choice when analyzing volatiles, but the perfumes complexity is very often too high to separate all target components in a single analysis. GC×GC-MS is the ideal tool match the complexity of the perfume samples thanks to its great peak capacity and enhanced sensitivity.

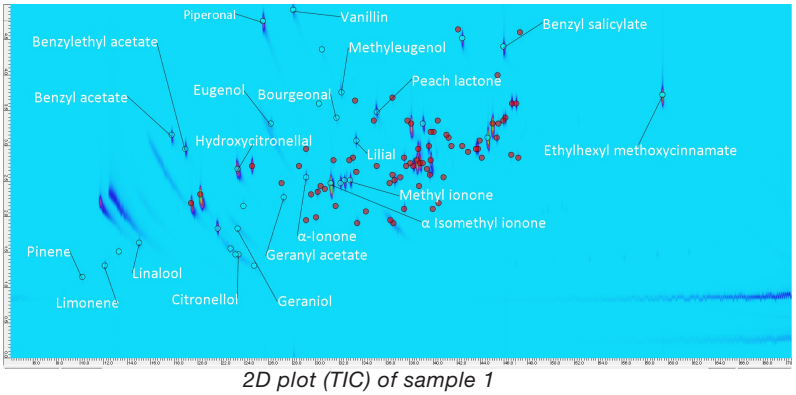
Samples

The samples were an eau de parfum (sample 1) and two eau the toilette (samples 2 and 3) of commercial brands purchased in a local store. These were analyzed directly.

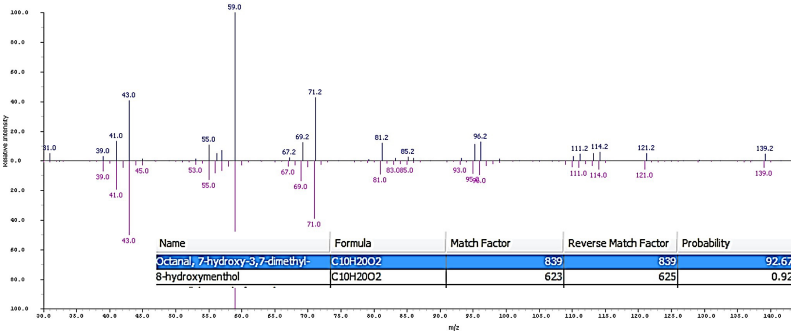
Instrumentation and software

All chromatograms were performed with an Agilent 7890B equipped with a Zoex ZX2 cryogen-free thermal modulator and an Agilent 5977A MS detector. All 2D data were displayed and analyzed using the Zoex GC Image software.

Results

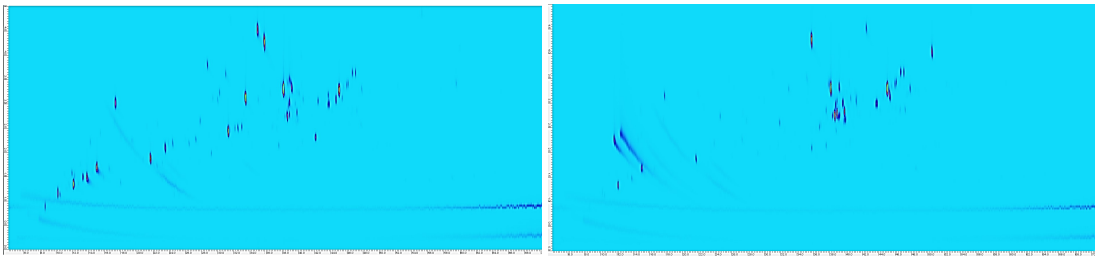


2D plot (TIC) of sample 1

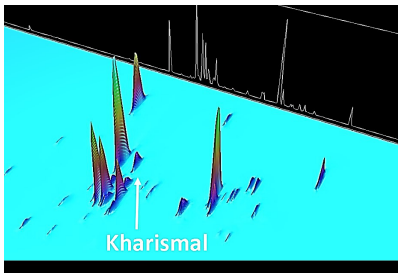


Mass spectrum for the allergen 7-hydroxy-3,7-dimethyl octanal (Hydroycitronellal) and relative match factor

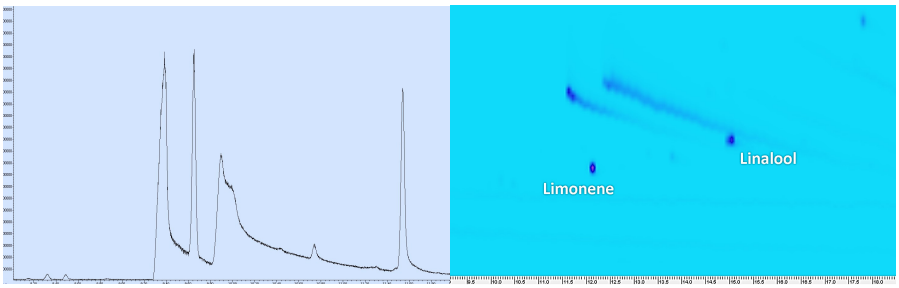
Over a hundred analytes are separated thanks to the high resolution power. This, combined with the good spectral quality, allowed identify more than 20 well-known aroma-key compounds and (suspected) allergens even when present in very small amount.



2D plots (TIC) of samples 2 (left) and 3 (right)



3D visualization of the GC×GC separation of an aroma compound from a complex chromatographic in sample 2



Example of allergens unresolved with GC-MS (left) and separated by GC×GC-MS (right) for sample 3

Major difference in fragrances/allergens. The (+) and (-) signs indicate that the compound is present or not, respectively.

Compound	Sample 1	Sample 2	Sample 3
Diethylphtalate	-	+	+
Vanillin	+	-	-
Y-decalactone	-	+	-
Eugenol	+	-	-
Hydroxycitronellal	+	-	-
Lillial	+	+	-
Benzyl benzoate	+	-	+
Helional	-	+	-
Ethlene brassyltate (*Musk T*)	-	-	+

Conclusions

- GC×GC-MS delivers a detailed separation of the fragrances.
- Several potential fragrance-key components and suspected allergens are identified.
- A chiral dimension would allow enantiomer separation. This would help correlating composition and fragrance and detecting fraud by differentiating natural and synthetic compounds.
- 2D plots can be compared by qualitative visual analysis, with minimal pre-processing and no need for identification.
- GC×GC-MS is a powerful tool for the chemical profiling of perfumes.

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