Advanced profiling of food volatiles by GC×GC-qMS: a comparative analysis of roasted hazelnuts from different origins ©

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Introduction

GC×GC combines an unmatched separation power with the capacity to generate highly ordered, structure-related patterns that help classification based on the analytes distribution in the 2D space. These features make GC×GC an excellent technique for the exhaustive characterization of complex samples such as those encountered in the food industry. The high level of detail obtained can be used for sample profiling, to identify signature markers responsible for flavor/taste, to evaluate different technological treatments, detect adulteration and guarantee authenticity. GC×GC-qMS is here used to compare and discriminate the volatile fractions of roasted hazelnuts from different varieties and geographical origin.

Experimental

Volatile components were sampled by HS-SPME and analyzed by GC×GC-qMS. All chromatograms were obtained by using GC×GC based on an Agilent 6890 equipped with a Zoex KT 2004 loop type thermal modulator coupled with an Agilent 5975 MS detector. 2D data were displayed and analyzed using the Zoex GC Image software.

Results summary

With the chromatographic fingerprinting approach 2D-peaks or 2D chromatographic regions are not identified and the attention is paid to the unique characteristics of the 2D plots. Thanks to the GC-Image software tools dedicated to advance fingerprinting (Image Investigator) a cumulative chromatogram of all samples is generated to identify all 2D regions with peaks to be used as distinctive features. These are compared to the individual samples chromatograms based on retention times and response intensity.

With the comprehensive template matching approach individual peaks (non-targeted or targeted) are individual features and the MS match factors are used to establish correct matching. Both methods use the features matching percentage to show (dis-)similarities between the samples.
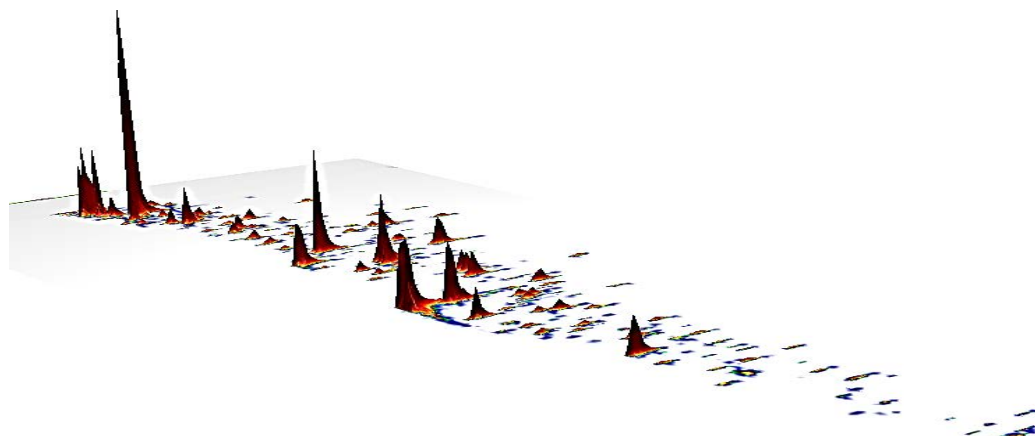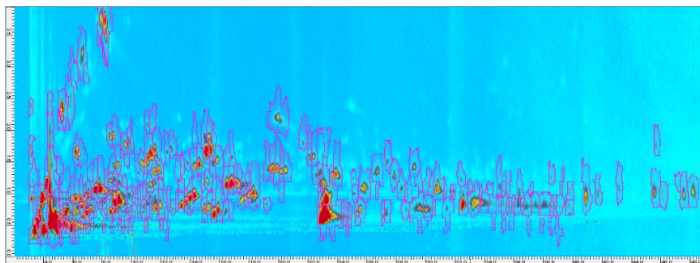
Chromatographic fingerprinting –
Cumulative chromatogram obtained for 9 hazelnuts samples. The pink polygons represent the region features adopted for samples classification.
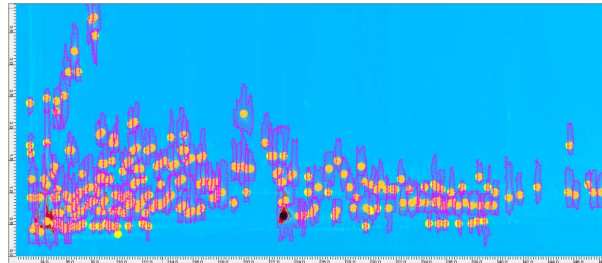
Comprehensive template matching –
The yellow dots represent matched compounds from a cumulative template of untargeted peaks (450 2D peaks).

	Ackakoca	Cile	Giffoni	Giresun	Mortarella	Ordu	Langhe	Romana	Trabzon
Ackakoca	0	75.7	75.0	64.7	71.3	81.6	56.6	64.7	80.1
Cile	73.2	0	69.0	69.7	63.4	76.1	52.1	58.5	71.1
Giffoni	71.3	68.5	0	40.6	78.3	70.6	63.6	67.1	83.9
Giresun	54.3	61.1	35.2	0	39.5	69.8	36.4	43.2	48.8
Mortarella	68.6	64.3	79.3	45	0	75.0	62.9	70.7	79.3
Ordu	54.4	52.9	48.5	54.9	51.9	0	35.9	45.1	52.4
Langhe	73.3	70.5	86.7	56.2	83.8	70.5	0	81.9	83.8
Romana	63.8	60.1	68.8	50.7	71.7	66.7	62.3	0	72.5
Trabzon	79.7	73.2	87.0	57.2	81.2	77.5	63.8	72.5	0

Matching % (or pattern similarity index) between samples obtained with template matching fingerprinting.
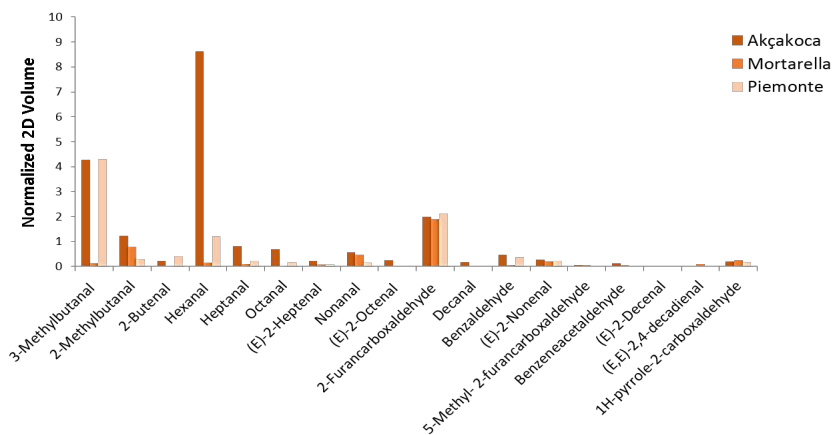
The discriminating peaks highlighted by the template matching can be used to build up signature-patterns of key-aroma compounds for the products based on their specific variety or geographical source.

Conclusions

- GC×GC can separate hundreds of different food VOCs analytes for detailed characterizations.
- Fingerprinting is an efficient method for general screening to find significant 2D differences.
- Template matching is more sensitive and specific thanks to the use of MS fragmentation to establish 2D peaks correspondences.
- Both methods successfully discriminate samples of different origin based on their quali-quantitative peaks distributions.
- The two approaches give consistent results.
- The approach is fully automatic and a dedicated software platform is available: Image Investigator

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