

Different data analysis approaches for the characterization of complex food matrices by GC×GC-qMS[©]

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Introduction

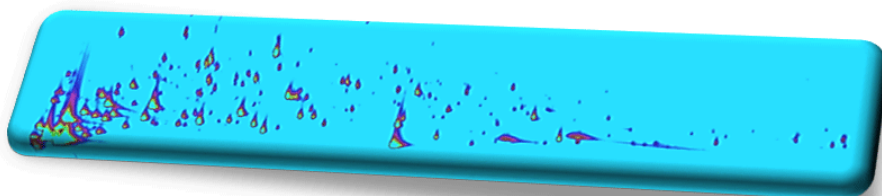
Safety and quality are subjects of ever-growing importance in food industry. A key aspect of food quality is the sensory impact due to flavor, smell and appearance. In fact some products have an added value thanks to quality labels based on specific origin and characteristic processing. This creates the need for analytical tools able to control precisely products with mandatory quality standard.

GC×GC-qMS is here used to analyze the highly complex volatile fraction of roasted hazelnut and coffee samples. The excellent separation obtained provides a large amount of valuable information and allows sample discrimination based on origin and roasting treatment.

Method

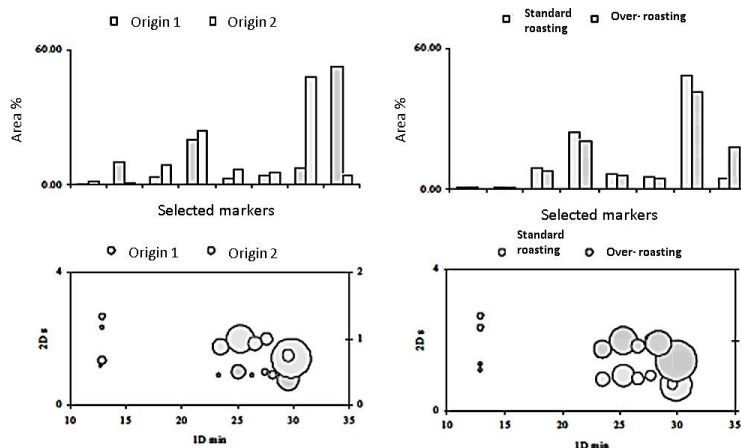
Volatile components were sampled by HS-SPME (DVB/CAR/PDMS fibers) and analyzed by GC×GC-qMS. All chromatograms were obtained by using GC×GC based on an Agilent 6890 equipped with a Zoex KT2004 loop type thermal modulator coupled with an Agilent 5975 MS detector. 2D data were displayed and analyzed using the Zoex GC Image software.

Results summary



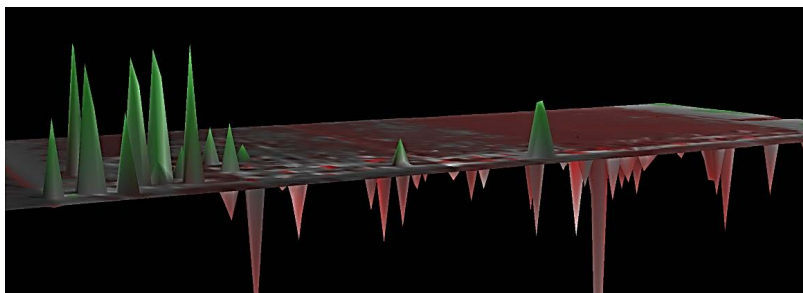
2D plot for a hazelnut sample.

1. Group-Type characterization: selected markers (target peaks) monitored in terms of relative % area over the total area of group members or normalized area versus an ISTD area.



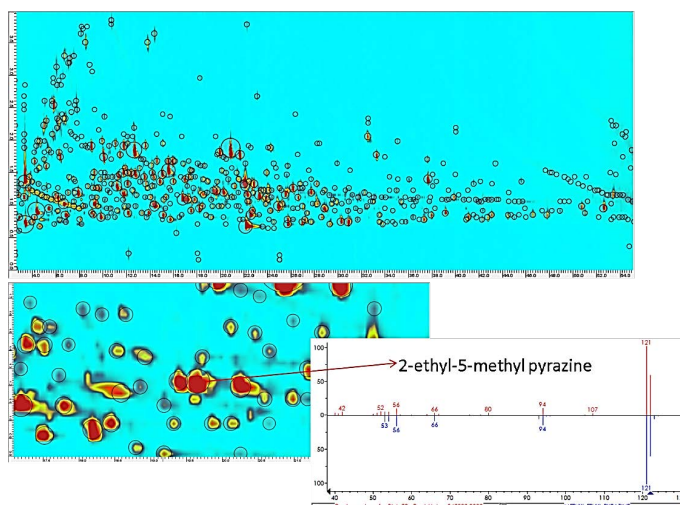
Example of group-type characterization for hazelnuts samples with furan compounds as selected markers.

2. Direct Fingerprinting by visual features: The 2D chromatograms are directly compared and compositional differences are shown visually. A dedicated software tool (GC Image) enables to correlate visual features with target analytes.



Differential image produced by comparing two hazelnut samples submitted to a standard treatment (reference - green) and over-roasting (red). The green and red peaks correspond to analytes present in larger and smaller amount.

3. Template Matching: A template of (non-) targeted 2D peaks built on a reference sample is adopted to establish correspondences between peaks of the same chemical entity (mass spectrum similarity constraint is optional). Aligned peak (meta) data is then used for comparative purposes.



Conclusions

- The high separation power of GC×GC unravels the sample complexity.
- Group-type characterization is easy and intuitive and does not need advanced software tools. Useful for qualitative and quantitative evaluations.
- Fingerprinting provides qualitative visual analysis with minimal pre-processing. No identification required. The MS response intensity gives semi-quantitative information.
- Template matching highlights the similarity degree (% of matching) on selected compounds/groups.

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