Chromatographic fingerprinting of hazelnuts volatiles by Comprehensive Two-Dimensional Gas Chromatography coupled with Time of Flight Mass Spectrometry: challenges in defining odorant patterns related to sensory defects

Federico Stilo;[1] Elena Gabetti;[1] Carlo Bicchi;[1] Nicola Spigolon;[2] Giuseppe Genova;[2] Marco Somenzi;[2] Mauro Fontana;[2] Chiara Cordero[1]

[1] University of Turin, Dipartimento di Scienza e Tecnologia del Farmaco (Turin, Italy)
[2] Soremartec Italia srl, (Alba, Cuneo Itay)

Abstract

The study of the composition of the volatile fraction (e.g., fingerprinting) encrypting the Chemical Odor Code[1], i.e., the chemical code of odor perception of a food, often poses severe challenges. Separation power and resolution enhancement, improved sensitivity and generation of structured separation patterns for groups of chemically correlated analytes are key-features that make comprehensive two-dimensional gas chromatography (GC×GC) a platform of choice to provide accurate and reliable results within *sensomic* workflows [2].

Raw hazelnuts connoted by sensory defects may show informative 2D patterns of volatiles that are diagnostic and helpful for their objective evaluation and quality assessment.

This study explores the potentials of high-informative fingerprinting on raw hazelnuts volatiles by combining head-space solid phase microextraction to GC×GC-tandem electron ionization- TOF MS. Hazelnuts of different geographical origin and cultivar, selected by flash-profile descriptive analysis for the presence/or not of sensory defects, are profiled and their 2D patterns processed by combined Untargeted and Targeted fingerprinting (*UT fingerprinting*) based on template matching principles.

UT fingerprinting performed at 70 eV EI data, merges targeted and untargeted reliable peak-features delineating patterns of analytes capable of clearly clusterize samples with *mouldy* notes, those with *rancid* and *solvent-like* odors.

Visual features fingerprinting[3] is here applied to create a "model peak-pattern" to be adopted as diagnostic probe for effective discrimination of defected hazelnuts.

References

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