

CHARACTERIZATION OF VOLATILE COMPOUNDS IN ITALIAN CIDER USING GC×GC-MS AND MULTIVARIATE ANALYSIS

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Cider is a traditional alcoholic beverage obtained by partial or complete fermentation of juice (fresh or reconstituted), with or without the addition of sugar, water or flavouring¹. In recent years, a global increase in its consumption has been recorded: this popularity may be related to the specific organoleptic profiles of ciders, which are closely associated with the variable contents of many aromatic compounds in the final beverage². One such group is commonly known as ‘volatile organic compounds’ (VOCs). Aroma profile, the utmost criteria in assessment of cider quality, is composed by many VOCs belonging to different chemical families³. Gas chromatography (GC) coupled with different detectors, such as mass spectrometry (MS) and flame ionization (FID) is the current technique for the robust analysis of VOCs. The complexity of most food matrices requires the isolation of the analytes as precursors before their introduction into the chromatographic system⁴. In this context, solid phase microextraction (SPME) offers considerable advantages. What is still not widely used in the characterization of VOCs in cider is the comprehensive two-dimensional gas chromatography^{5,6}. The aim of this work is the characterization of different Italian ciders by HS-SPME-GC×GC-ToFMS. Multivariate statistical approaches play a crucial role, allowing to extrapolate meaningful information from the data. After building the clean dataset of the analysed VOCs, three other datasets were obtained, normalized respect to the three internal standards used (Acenaphthene-d₁₀, 1,4-Dichlorobenzene-d₄, Naphthalene-d₈), to evaluate their influence on the analytical method. These datasets have been analysed with main unsupervised methods of Machine Learning, Principal Component Analysis (PCA), Cluster Analysis (CA) and t-distributed Stochastic Neighbor Embedding (t-SNE), which made it possible to highlight the robustness of the method, showing similar results for the different datasets. Moreover, the exploratory analysis allows to identify different classes of ciders, which are distinguished by the fermentation process or the addition of flavouring, such as hops.

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