MULTIVARIATE ANALYSIS OF COMPREHENSIVE TWO DIMENSIONAL GAS CHROMATOGRAPHY AND TIME-OF-FLIGHT MASS SPECTROMETRIC DETECTION DATA FOR DIFFERENTIATION WINES

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Aroma is one of the most important factors in determining wine character and quality. The aroma characteristics are the result of complex interactions among four factors: vineyard geographical site, which it is related with the soil and climate characteristics, grape variety, yeast strain, and technical conditions of wine-making. The objective of this study was to determine the volatiles that characterize and differentiate wines produced with red or white grapes. A headspace solid-phase microextraction (HS-SPME) combined with comprehensive two-dimensional gas chromatography-time-of-flight mass spectrometry detection (GC×GC/TOFMS) was used to analyze the volatiles in four types of wines elaborated with red grapes (Cabernet Sauvignon and Merlot) and white grapes (Chardonnay and Sauvignon Blanc). Fisher ratio and principal component analysis (PCA) were used to determine the volatiles related to each wine group. The wines elaborated with red grapes are characterized by furfural, dihydro-2(3H)-thiophenone, octanal, tetradecanal, 5-hexylidihydro-2(3H)-furanone, geranic oxide, \(\beta\)-damascenone, tetrahydro-2H-pyran-2-one and 2-phenylethylacetate, 2-ethylpentanal, propan-2-one, 6-methylpentan-1-ol, 1,4-butanediol, 1-hexanol, 5-(hydroxymethyl)furan-2-carbaldehyde and ho-trienol. Only esters including ethyl dodecanoate, ethyl octanoate, isoamyl octanoate, 3-methylbutyldecanoate, ethyl pentanoate, ethyl lactate and isoamyl lactate were the compounds that differentiated the wines produced with white grapes from those produced with red grapes. A detailed examination of GC×GC/TOFMS data demonstrated that some of the twelve most important volatiles co-eluted with other compounds and would not be identified only with the use of one-dimensional gas chromatography. Theses results may be useful for differentiation of wines from different varieties and establishing criteria to improve the quality of the wines.