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Optimization and validation of a DHS-TD-GC-MS method to wineomics studies

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Abstract

A dynamic headspace sorptive extraction (DHS) combined with thermal desorption (TD) and coupled with gas chromatography-mass spectrometry (GC/MS) was developed for the determination of forty-four volatile aroma metabolites (VAMs) which describe aroma fingerprints of wines. The response surface methodology (RSM) and a central composite design (CCD) was used to obtain the optimal values for the experimental extraction variables, and the results were assessed by an analysis of variance (ANOVA) and a principal component analysis (PCA). The VAMs exhibited optimal extraction with the high levels of salt concentration (1.5 g NaCl) and using an extraction temperature of 40 ºC during 10 min, and a subsequent purge volume of 300 mL. Subsequently, the calibration curves were created for the quantification of each VAMs with seven levels of concentration obtaining a correlation coefficients (R^2) above 0.9900 for all of them. The proposed method was successfully validated and showed good precision and accuracy values for all VAMs. Lastly, the method was applied to quantify VAMs, responsible for the aroma fingerprints of white and red wines, from different Denomination of Origin

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