

Simultaneous determination of toxic compounds produced during fermentation of wine

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The analytical laboratories have demonstrated increasing interest in the use of methods to quantify more than one compound in a single analysis, as a way of reducing the sample preparation time and, consequently, the total analysis time and also as a way to reduce costs. The *gas chromatography with mass spectrometry detection* is the most used technique in the determination of volatile compounds. Recently, the comprehensive two-dimensional gas chromatography (GC×GC) has been used in the determination of multi-compounds from complex samples because this technique enhances the separation of the analytes from each other and the in relation to other components of the matrix, among other advantages. The objective of this study was to investigate the need to use of GC×GC to quantify toxic compounds (acetaldehyde, formaldehyde, ethyl carbamate and acrolein) produced during the fermentation of Syrah wine. The four toxic compounds were simultaneously extracted by headspace solid phase microextraction after derivatization of the sample with 2,2,2-trifluoroethylhydrazine. The GC×GC proved to be an important tool for the quantification of acetaldehyde and acrolein, since these compounds coeluted with other compounds in the first dimension (¹D). Acrolein, for example, coeluted with methyl hexanoate (retention time in the second dimension, ²T_R = 4,13s) and 3-methyl-1-butanol propanoate (²T_R = 4.79 s) in ¹D (retention time in the first dimension, ¹T_R = 14.81 min). Acetaldehyde (²t_R = 2.17s) coeluted with limonene (²T_R = 5.84s) and ethyl 4- methyl pentanoate (²T_R = 4.70s) in ¹D (¹T_R = 14.93 min). Figures of merit of the method were: recoveries from 90.4 to 102.2 % and repeatability from 1.8 % to 15.8%. LOD was 0.005 µg L⁻¹ for acrolein, 0.03 µg L⁻¹ for ethyl carbamate, 0.1 µg L⁻¹ for formaldehyde and 10 µg L⁻¹ for acetaldehyde. The combination of GC×GC/TOFMS for quantitative analysis of volatile toxic compounds found in wines have shown to be advantageous and may facilitate the implementation of a quality control for the wine industry.

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