OC40: FTIR-ATR and FDA applied as chemometrics techniques to distinguish ageing processes of wine spirits

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The contact of the wine distillate with the wood is recognized as a fundamental step in the production of aged wine spirit, during which its quality increases. In this study, functional data analysis (FDA) was applied to spectral data collected in Fourier transform infrared spectroscopy (FTIR) with Attenuated Total Reflection (ATR) to differentiate aged distillates produced in 250 L wooden barrels *versus* produced in 1000 L stainless steel tanks with wood staves. The aim of this study is to examine the effectiveness of an easy and fast tool to identify the different ageing processes of wine spirits over the time (up to 18 months). For this purpose, FDA was applied to the data of low molecular weight compounds of wine distillates collected by HPLC and by FTIR-ATR. The low molecular weight phenolic acids (gallic acid, vanillic acid, syringic acid and ellagic acid), phenolic aldehydes (vanillin, syringaldehyde, coniferaldehyde, and sinapaldehyde), coumarins (umbelliferone and scopoletin), and furanic aldehydes (5-hydroxymethylfurfural, 5-methylfurfural, and furfural) were quantified by HPLC according to the method of Canas et al. (2003).[1] FTIR-ATR Spectra were acquired in the selected region identified in Figure 1 with a Bruker spectrometer (Alpha, Bruker Optic GmbH,Ettlingen, Germany) using a diamond crystal according the methodology described by Anjos et al. (2016).[2] FDA was performed according to the method previously described in Anjos et al. (2020).[3] The results show that FDA applied to spectral analysis allows discriminating samples of wine spirits with different ageing time and aged with different kinds of wood. It is also possible to distinguish between traditional and alternative ageing processes used in the ageing process. In conclusion, the applicability of these chemometric techniques to correlate the analytical determination of low molecular weight compounds and the FTIR-ATR/FDA in differentiating aged wine spirits by different modalities is proven.

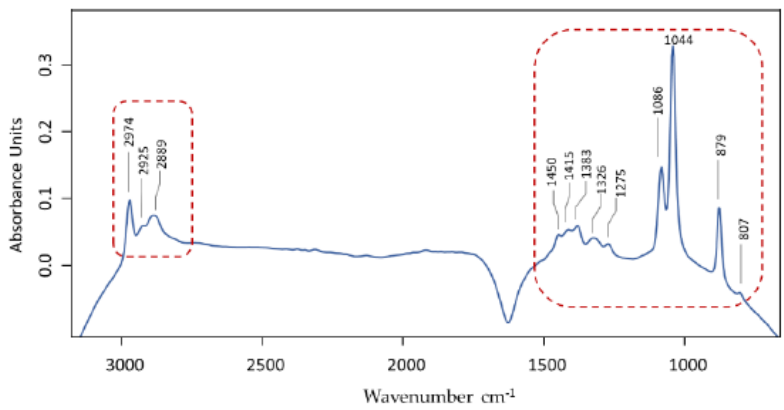

Figure 1. FTIR-ATR absorbance spectra of wine spirit samples with the more representative region marked.

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