

## PC-D07: FTIR-ATR, FT-RAMAN and GC-FID assessment of discrimination of aged wine spirits under different conditions

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Spectroscopic techniques namely Fourier transform infrared spectroscopic with attenuated total reflectance (FTIR-ATR) and FT-RAMAN can be powerful tools to assess the quality of many different foods and beverages.<sup>1,2</sup>

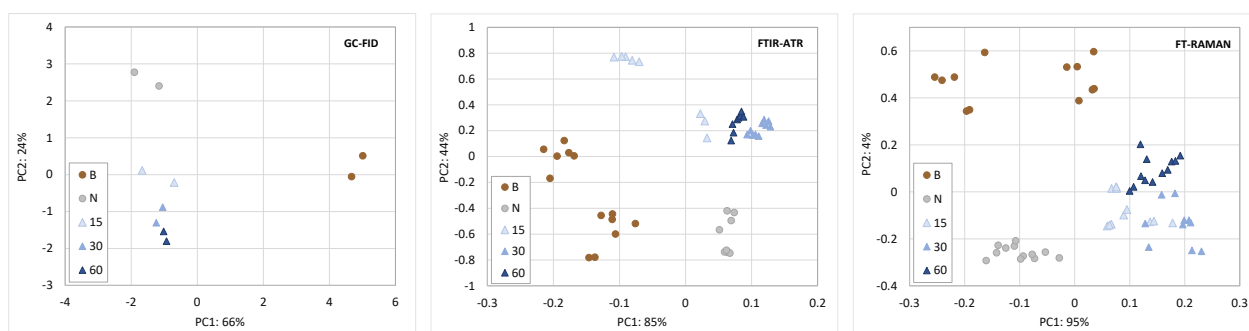
The aim of this work was to evaluate the performance of FTIR -ATR, FT-RAMAN and GC-FID to discriminate wine spirits aged with chestnut wood during one year in 250 L wooden barrels and in 50 L demijohns with staves combined with different micro-oxygenation levels.

Different approaches were used to evaluate the differences between the wine spirits resulting from the ageing modalities studied. The first one was the application of GC-FID for the quantification of odorant compounds in the wine spirits.<sup>3</sup> The second one was the evaluation by spectroscopy techniques, specifically FTIR-ATR and FT-RAMAN.

GC-FID analysis was performed in a chromatograph (Agilent Technologies 6890N) equipped with fused silica capillary column of polyethylene glycol (HP-INNOWax, Agilent Technologies, Palo Alto, CA, USA), 30 m, 0.32 mm i.d., 0.25  $\mu\text{m}$  film thickness, under the chromatographic conditions described by Caldeira *et al.* (2021).<sup>3</sup>

FTIR-ATR spectra were acquired in a Bruker FTIR spectrometer (Alpha) with a resolution of 4  $\text{cm}^{-1}$  in the wavelength region 4000-400  $\text{cm}^{-1}$ , using a diamond single reflection attenuated total reflectance (ATR). All spectra were obtained with 32 scans. The FT-RAMAN spectra were acquired using a FT-RAMAN spectrometer (BRUKER, MultiRAM) with a spectral resolution of 4  $\text{cm}^{-1}$ , scanner velocity of 5 KHZ and 100 scans per sample. All spectra (from FTIR-ATR and FT-RAMAN) were collected at a constant room temperature of 20 °C.

ANOVA results showed a significant effect of the ageing modality on the contents of volatile compounds, namely linalool, acetic acid, syringol and ethyl acetate. Regarding the principal component analyses performed with the results from the three methodologies, it was found a clear separation of the aged spirit samples based on the technology used in the ageing process (**Figure 1**).



**Figure 1:** Principal component analysis of GC-FID, FTIR-ATR and FT-RAMAN of wine spirits samples from different ageing modalities

Great differentiation of the volatile composition between samples from alternative ageing processes and those from the traditional process in wooden barrels was observed. This differentiation was also found by the spectroscopy techniques applied, with more accurate results observed for RAMAN. These outcomes show that FTIR-ATR and FT-RAMAN are powerful techniques for the quality control of wine spirits, since they allow a quick discrimination between samples produced with different methodologies.

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**References:**

1. O. Anjos, A.J.A. Santos, L.M. Estevinho, I. Caldeira, Food. Chem. (2016) 205:28–35.
2. O. Anjos, M.G. Campos, P.C. Ruiz, P. Antunes, Food. Chem. (2015) 169:218–223.
3. I. Caldeira, C. Vitória, O. Anjos, T.A. Fernandes, E. Gallardo, L. Fargeton, B. Boissier, S. Catarino, S. Canas, Appl. Sci. (2021) 11: 3991.