

# Livro de Resumos

## XV Encontro de Química dos Alimentos



MADEIRA

ENCONTRO DE  
QUÍMICA DOS  
ALIMENTOS

5-8 DE SETEMBRO DE 2021



ESTRATÉGIAS PARA A EXCELÊNCIA,  
AUTENTICIDADE, SEGURANÇA  
E SUSTENTABILIDADE ALIMENTAR



SOCIEDADE PORTUGUESA DE QUÍMICA



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# Comunicações em Painel

*PC-D: Química alimentar*



# Comunicações em Painel

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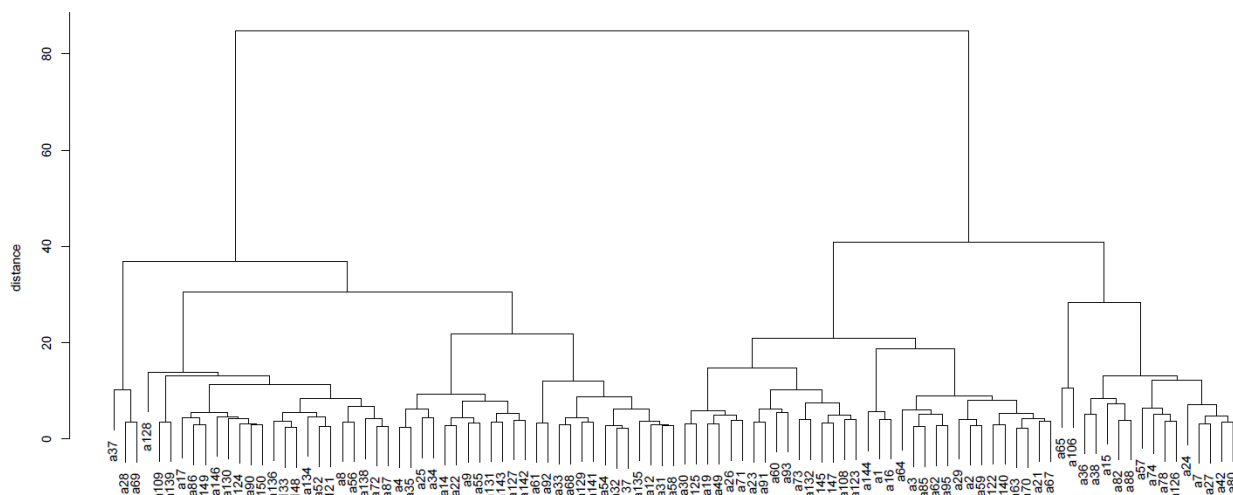
## PC-D34 FTIR-chemometric analytical methodology as a tool for clustering oils from centenarian olive trees grown in the Côa Valley region

**Pascoal-Ferreira P, Peres AM, Silva K, Santamaria-Echar A, Barreiro F, Pereira JA, Baptista P, Rodrigues N**

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The centenarian olive trees are part of the historical and cultural heritage of the Côa Valley region where a significant number of these specimens can be found. They have high importance in olive grove heritage; however, their genetic and phenotypic diversity is still poorly studied. The identification of olive tree varieties is not an easy task, being required a morphological characterisation complemented with genetics, making this identification a time-consuming and expensive procedure. Recently, Fourier Transform Infrared (FTIR) spectroscopy start to be widely used in several studies in the food field, becoming a powerful analytical tool for the analysis of edible oils and fats<sup>1</sup>. This technique has numerous advantages, allowing a fast and non-destructive analysis, and requiring minimal sample preparation. In this context, FTIR has been applied to classify and identify different fats<sup>2</sup>, detection of virgin olive oils adulteration<sup>3</sup>, determination of trans fatty acids<sup>4</sup> and evaluation of oil mixtures<sup>1</sup> composition in foods<sup>5</sup>, all this based on the spectral profiles<sup>6</sup>. Considering that there is a great diversity of centenarian olive trees in which the varieties are unknown, the objective of this work was to use the FTIR technique to identify groups of olive oils with similar chemical characteristics, thus reducing the time and required amount of samples for analysis. Therefore, FTIR was applied to 99 olive oils from centenarian olive trees in the Côa Valley region. FTIR analysis was carried out using an MB300 FTIR from ABB (Zurich, Switzerland) operating in attenuated total reflectance (ATR) mode using a horizontal cell equipped with a diamond crystal. The spectra acquisition was done using 32 scans/min at a resolution of 4 cm<sup>-1</sup>, being the reading range comprised between 4000 and 500 cm<sup>-1</sup>. Spectra were acquired and treated using the software Horizon MB version 3.4. The background was acquired every two consecutive assays. Finally, raw transmittance data (in %) of the different olive oils were used for the statistical analysis. A hierarchical clustering dendrogram was applied to evaluate the possibility of grouping the 99 olive oils studied according to the full FTIR spectra by computing the distance (dissimilarity) among the olive oils, using the Euclidean distance Ward method for matrix computation. The dendrogram (Figure 1) allowed identifying dissimilarities based on the olive oils' FTIR spectra, enabling to establish 4 main clusters, for a 2<sup>nd</sup> node cut establishing responding to a distance around 35. Since FTIR spectroscopy is sensitive to different aspects including the olive variety and considering that all the olive oils were extracted under similar conditions and from olives harvested in the same geographical regions, the observed variations can be tentatively attributed to the olive variety or to a similarity of the oils' chemical composition. The clustering analysis allowed partitioning a large dataset of olive oils into smaller groups based on similar spectra characteristics, enabling the future practical and feasible evaluation of selected oils belonging to each of the 4 established clusters, avoiding the need to evaluate each one of the 99 olive oils.



**Figure 1:** Hierarchical clustering dendrogram (using Euclidean distances and Ward method), based on the FTIR spectra ( $4000 - 500 \text{ cm}^{-1}$ ) recorded during the analysis of 99 olive oils extracted from olives harvested from centenarian olive trees located in the Côa Valley region.

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