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Data Article

Data on fatty acid profiles of green Spanish-style Gordal table olives studied by compositional analysis



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ABSTRACT

This article contains processed data related to the research published in “Tentative application of compositional data analysis to fatty acid profiles of green Spanish-style Gordal table olives” (Garrido-Fernández et al., 2018) [1]. It provides information on the implementation of compositional data analysis (CoDa) to the fatty acid profiles of Spanish-style Gordal table olives vs the use of conventional statistical analysis (data composition expressed in percentages). Particularly, it includes: i) the matrix of the sequential binary partition used for the balance estimation and the isometric log-ratio transformation (*ilr*) of the fatty acid profiles, ii) correlation among the diverse fatty acids expressed in percentages and their significances, iii) the *ilr* transformed values (*coordinates* in the Euclidean space) obtained following the sequential binary partition previously detailed, iv) the graphical presentation in the Simplex (ternary centred plot) of the treatments as a function of the four fatty acids with the higher log-ratio variances, and v) segregation of treatments based on Cluster Analysis.

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Specifications Table

Subject area	Chemistry
More specific subject area	Food Chemistry
Type of data	Tables, Figures, Text file
How data was acquired	Fatty acid profiles were acquired by analysis of their methyl esters (FAMES) in a Hewlett-Packard 5890 series II gas chromatograph
Data format	Raw, filtered and analysed data
Experimental factors	Processing phases of green Spanish-style Gordal table olives and fat extraction systems
Experimental features	The design consisted of 5 replicate treatments. Three processing phases (fresh, fermented, and packaged olives) plus two extraction systems (Abencor and Soxhlet)
Data source location	Seville, Spain, 37°21'36.5''N; 5°56'18.6''W
Data accessibility	The data are available with this article

Value of the data

- The data include the sequential binary partition of fatty acid profiles in CoDa and could be useful for calculating balances and the *ilr* transformation for other food compositions and interested researchers.
- The correlation among fatty acids expressed in percentages may help other researchers for finding spurious relationships.
- The information may facilitate the comparison of conventional multivariate techniques and compositional, regardless of the field, and promote international collaborations in data analysis.
- Presentation in the Simplex can be an appropriated way of graphing compositional data and treatments' effects.

1. Data

The data cover aspects of conventional and compositional analysis. Particularly, the presentation of these data in the Simplex (Fig. 1), the binary partition (Table 1), the *ilr* transformations based on it (Table 3) as well as the application of multivariate tools to the original data (Table 2 and Fig. 2A) and *ilr* coordinates (Fig. 2B).

2. Experimental design, materials and methods

Olives (maturity index=1) [2] were processed in duplicate according to the green Spanish-style. After fermentation for eight months, 10 kg olives from each replicate, were packaged in glass containers (50 g NaCl/L and 5.5 g lactic acid/L cover brine), stabilized by pasteurization, and stored at room temperature (22 ± 2 °C) for two months. The applied processing and packaging mimicked those used at industrial scale [3]. Samples (~5 kg olives) were withdrawn in duplicate from i) the fresh Gordal olives extracted by Abencor (RM), ii) each of the replicates of the fermented fruits (extracted by Abencor (FO) and Soxhlet (FOS)), and iii) packaged olives (extracted by Abencor (PO) and Soxhlet (POS)). The olives from the samples were pitted, homogenized with an Ultra-Turrax T25 (IKA-Labortechnik, Staufen, Deutschland) and extracted as described elsewhere [4,5].

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