# Livro de Resumos

# XV Encontro de Química dos Alimentos


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# Comunicações em Painel

## *PC-D: Química alimentar*

# PC-D42: The use of the FTIR as a tool to discriminate flavoured oils

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Olive oil is one of the most consumed vegetable oils in the world, and its production has been increasing in recent years. However, in the last decade there has been a demand for new products by consumers. Thus, the industries together with the market have been trying to create new products or reactivate products with a long tradition to create and revive sensations, as is the case with flavoured oils. New products have emerged with the addition of traditional aromas and flavours, and also with the inclusion of differentiated aromas as well as different forms of incorporation[1]. Most of the flavouring agents used are aromatic herbs and spices (e.g., chili pepper, pepper, lavender, bay leaves, garlic, rosemary, basil, thyme, oregano), fruits (e.g., lemon, orange). However, flavoured oils cannot be labelled with the usual commercial grade terminology (i.e., extra virgin or virgin olive oil)[2]. Thus, to avoid the risk of mislabelling, there is a need to develop fast, low-cost and non-invasive analytical techniques that allow identifying the flavouring agent as well as to discriminate unflavoured from flavoured oils. In this context, techniques based on spectroscopy have gained great importance as they allow a fast non-destructive analysis using a small volume of oil. Indeed, Fourier transform infrared spectroscopy (FTIR) has been used as a tool to track and authenticate foods, having served as the basis for detecting adulteration in olive oil[3], assessing oil's oxidation level[4], identifying the commercial category of the oil[5], determining the sensory intensities as well as for recognizing the oil's geographic origin [6]. So, this study reports the use of FTIR coupled with chemometrics to discriminate unflavoured (control) and flavoured olive oils (with cinnamon powder, garlic powder and dried rosemary). Oils were flavoured in a proportion of 1.5% w/v and stored at dark and ambient temperature, in amber glass bottles (4 independent bottles for each oil) during fifteen days, to promote the flavouring process. After that, the oil of each bottle (16 bottles in total) was filtered and spectroscopically analysed in triplicate. The raw spectra were recorded between 4000-500 $cm^{-1}$. Raw transmittance data (in %) as well as the respective 1$^{st}$ and 2$^{nd}$ derivatives (Figure 1) were used to establish the most powerful linear discriminant (LD) models, based on selected non-redundant wavenumbers (identified using the simulated annealing meta-heuristic variable selection algorithm, SA) among those belonging to the absorption regions (3150-2500 and 1700-600 $cm^{-1}$). The study revealed that both raw and transformed data could be used to successfully discriminate the olive oils under study, allowing the LD-SA-FTIR models a correct classification (100% sensitivity) of all samples for the original grouped data (Figure 2) as well as for the leave-one-out cross-validation procedure. The predictive performance of the classification models was further evaluated based on the repeated K-fold cross-validation procedure, in which, the initial data matrix was split into 4 folds (K=4 in this study), allowing to use 25% of the data for internal validation purposes, being the random split repeated 10 times. The results showed that the models could correctly classify 98, 100 and 100% of the samples based on the raw, 1$^{st}$ derivative or 2$^{nd}$ derivative models, respectively. These results demonstrated the potential use of the FTIR-chemometric approach as an authentication tool for flavoured and unflavoured olive oils.

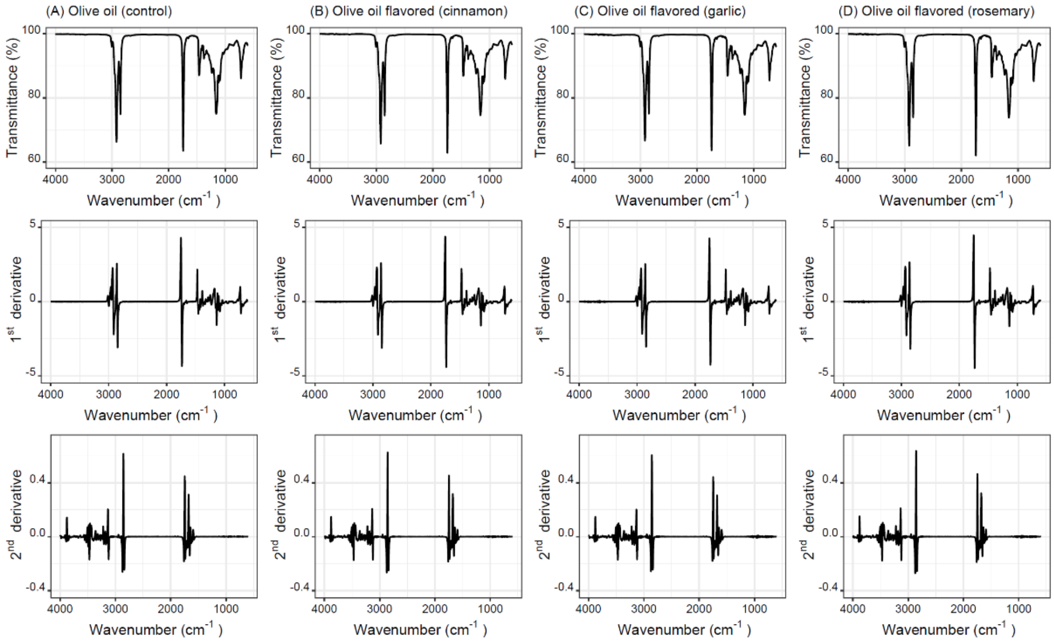


**Figure 1**: FTIR spectra (4000 to 500 cm$^{-1}$) and respective 1$^{st}$ and 2$^{nd}$ derivatives for unflavoured and flavoured olive oils of: (A) Unflavoured oil (control); (B) Oil flavoured with cinnamon powder; (C) Oil flavoured with garlic powder; and, (D) Oil flavoured with dried rosemary.

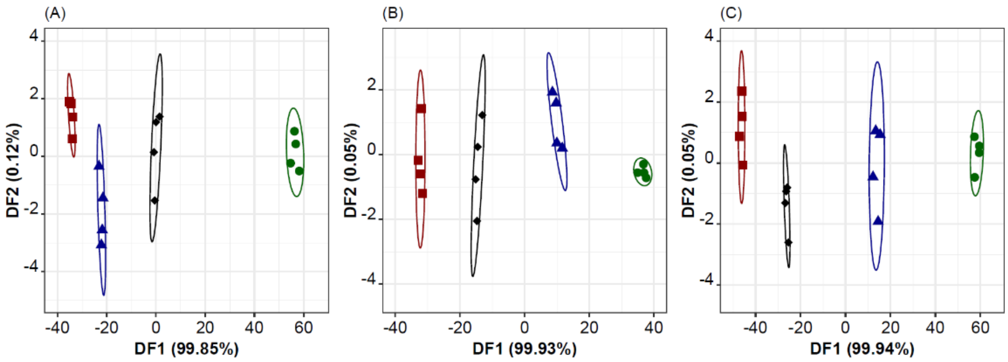


**Figure 2**: Olive oils supervised discrimination (●: Oil flavoured with cinnamon powder; ▲: Unflavoured oil (control); ■: Oil flavoured with garlic powder, ♦: Oil flavoured with dried rosemary): (A) LD-SA-FTIR raw data model based on 5 wavenumbers (1269, 845, 827, 696, 667 cm$^{-1}$); (B) LD-SA-1$^{st}$ derivative FTIR model based on 5 wavenumbers (3126, 2953, 905, 847, 808 cm$^{-1}$); and, (C) LD-SA-2$^{nd}$ derivative FTIR model based on 5 wavenumbers (2924, 2912, 1695, 839, 744 cm$^{-1}$).

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