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Towards Neutron Scattering Identification of Olive Oil’s Antioxidant Properties

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Extra virgin olive oil (EVOO) is one of the most important ingredients as well as the main source of lipids in the Mediterranean diet. It is known to contain bio- logically relevant phenolic components with recognized health-beneficial properties. For this reason, EVOO is defined as a functional food with high antioxidant and anti-inflammatory capacity. These characteristics de- pend on the structural and conformational behavior of the phenolic components, namely phenolic acids and esters, for example, cinnamic acid derivatives, which are largely determined by intra- and intermolecular H-bond interactions. Moreover, the amount of these compounds in EVOO may vary depending on several factors, such as olive cultivar, location, climate, degree of maturation, agronomic and technological aspects of production. Following the protective role of such minor phenolic components against carcinogenesis, a direct relationship has been found between the EVOO consumption and the incidence of different types of cancers and chronic non-communicable diseases [1].

The study of the vibrational dynamics of the phenolic components within olive oil can be a source of insightful information, such as the formation and chain length of alkyl esters and the presence of intermolecular hydrogen- bond interactions, inducing the dimerization of esters, thus shedding light on their structure–activity relationship. For this reason, inelastic neutron scattering (INS) and Raman spectroscopy have been used in the past to investigate isolated phenolic compounds. However, their application to real-life samples is more challenging, for the signal from these minor compounds is generally overwhelmed by the one from triacylglycerols and unsaturated fatty acids, such as CH_2 vibrations at about 750 and 1300 cm^{-1}.

In this framework, the results recently published [2] aimed to assess possible strategies for the application of vibrational techniques to investigate the spectroscopic fingerprints of minor phenolic compounds in EVOO samples. The EVOOs considered in this study were commercially available with origins from olives organically or bio-organically grown within the Italian regions of Toscana, Umbria, Puglia, Lazio, and Abruzzo. By comparison with the spectra from hydroxytyrosol and other minor phenolic compounds, two regions were recognized as the most promising to look for information regarding the structure–activity relationship: the energy regions around 675 and 1200 cm^{-1} for the signal from hydroxytyrosol, and around 450 cm^{-1} for all minor phenolic components used as reference. Moreover, it was noted that, by using a selectively deuterated sample, the slightly structured signal from the major components in these regions could be additionally suppressed, making the analysis of the minor phenolic components easier.

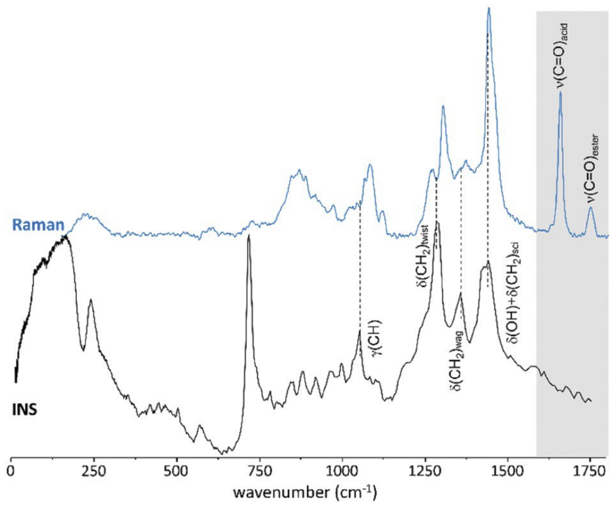

Figure 1. INS and Raman spectra (0–1750 cm^{-1}) of one of the extra virgin olive oil samples studied, with emphasis on the vibrational modes at 1655 and 1745 cm^{-1}, corresponding to acid and ester vibrations, respectively. Figure adopted from Senesi *et al*. [2].

Moreover, when comparing neutron and Raman data, differences in EVOO samples investigated appeared to be mostly related to the different amounts of phenolic esters versus acids. This feature was reflected by the relative intensities of the peaks at 1655 and 1747 cm^{-1} in the Raman data, as shown in Figure 1. The latter peak was not found in either the secoiridoids or hydroxytyrosol constituents taken as reference. Following a detailed analysis of the Raman features of the carbonyl stretching modes, differences in the relative concentrations of acids and esters were related to the regional origin of the EVOO samples. Also, all EVOO samples were found to have a higher relative intensity from phenolic esters than a reference sample of sunflower oil [3].

In conclusion, the characterization of the predominant signal from major components in EVOO is a fundamental step toward the investigation of the spectroscopic fingerprints from minor phenolic components. These results are likely to facilitate future experiments, using both INS and Raman spectroscopy, on real-life EVOO samples, possibly using selective deuteration. In the case of neutron techniques, the knowledge of the vibrational spectrum may allow energy-selective neutron imaging experiments [4].

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