Raman spectroscopy in the evaluation of different oleogels types

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Oleogel is a promising alternative that can be incorporated into different health food as a conventional fat replacement. The oil type is a key factor when determining technological properties and choosing applications since they are exclusive in their fatty acid composition, atomic weight, and thermal characteristics, which influences the gelation capacity. Therefore, this work aimed to analyze and classify these oleogels in a fast reliable way (free of chemicals) using Raman spectroscopy. Raman spectroscopy is a rapid detection technique and provide a structural fingerprint. It can be used to characterize and identify cis and trans isomers, as well as analyze the structure and classification of oils. Three oleogels were prepared with 95% of oil (sunflower, soy, olive), and 5% of bee wax as structuring agent, melted at 90 °C. Official methods were used to access the fatty acid composition of peroxides and free fatty acids. Rheology analyzes were also conducted to aid in classification. A total of 240 spectra were acquired 0.5 cm from the sample. The spectra were collected in a range of 785 - 1065 nm and the laser power was 300mW. After spectra pretreatment, PCA was performed and it was possible to observe the sample clustering for each oil type in the PC scores. Classification models were then performed using the full dataset with samples split in calibration set 70% (162 samples) and validation 30% (78 samples). The best SIMCA model classified with 98% of accuracy; some samples of olive oil were misclassified to sunflower oil. PLS-DA reached better performance than SIMCA, classifying samples with 100% of accuracy, demonstrating that a portable Raman spectrometer in tandem with chemometrics can be a promising tool to classify different types of oleogels.