Raman Spectra acquisition of Extra Virgin Olive and Sunflower oil mixtures

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1. Context

The purpose of the Dataset is to define a predictive model to estimate Extra Virgin Olive Oil percentage in an Olive and Sunflower oil mixture. Data set was use in Partial Least Squares Model.

2. Raman Set Up parameters:

Raman spectrometer QEPro (Ocean Insight, USA) set up for 785 nm with a Raman Shift: from 500 cm^{-1} to 2500 cm^{-1}, a typical optical resolution of 11 cm-1 full width at half maximum (FWHM) and an integration time of 1000 ms. For all resulting spectra 10 scans were done for each acquisition. A Solid-state laser diode (Ocean Insight, USA) with an excitation wavelength of 785 nm was used with a power of 400 mW and a spectral FWHM inferior to 0.15 nm. A a general-Purpose Fiber Optic Raman Probes (Ocean Insight, USA) was used with a specific quartz cuvette holder with a working distance of 0.5mm. In accordance with our Design of Experiment 5 spectra were recorded with each mixture.

3. Sampling

The document is a series of 605 Raman Spectra of different mixtures of Extra Virgin Olive Oil (EVOO) and Sunflower oil.

Samples are mixture of Extra Virgin Olive Oil (EVOO) and Sunflower oil and are classify from 0 to 100% EVOO. EVOO is 100% Italian cold pressing extra virgin olive oil bottled in Italy for the trademark PUGET; The EVOO had an acidity of 0.3%a and an unsaturated fat content of 14 g/100 g. Sunflower oil is a refined oil from Spain (Trademark FAIGES) with an acidity of 0.2%, an unsaturated fat content of 10 g/100 g and a vitamin E content of 80mg.

4. Data set organization

The Data set have 605 Raman spectra and it is organized with the following structure.

Column A	Acquisition date
Column B	Observation number for a same date
Column C	Spectrum number for the same mixture
Column D	Percentage of EVOO
Column E	Percentage of Sunflower oil
Column F	Acquisition time in ms
Column G	Number of scans
Column H	Laser Power in mW
Column I	Data set origin CALIBRATION, VALISATION or PREDICTION
Column J to AAQ	Raman intensities for different wave numbers from 500 to 2500 cm^{-1}