Evolutionary computational based methods and spectral data analysis A case study: Adulteration of olive oil

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The authentication of extra virgin olive oil and its adulteration with lower quality oils are serious problems in the olive oil industry. In addition to the obvious effect on the producer profits, adulteration can also cause severe health and safety problems. A number of techniques, including chromatographic and spectroscopic methods, have been employed to assess the purity of olive oils. In particular, the use of vibrational spectroscopy in combination with chemometrics (e.g. partial least square regression algorithms and analytical neural networks) has been shown to predict successfully the composition of a given oil mixture. However, whilst it can be argued that quantitative results obtained from PLSR and ANNs are excellent, the models produced are not easily interpreted; that is to say, it is not obvious how these methods exploit information specifically in terms of the values of the different input variables (e.g. absorbance or Raman shifts). Evolutionary computation may provide further information thereby allowing chemical deconvolution of the spectra.

In this study Raman spectroscopy (spectra were collected with a Renishaw System 100 Raman spectrophotometer with a near infrared 780nm laser with the power at the sampling point typically at 20mW) together with evolutionary computational methods has been employed to quantify the amount of adulterant oils, such us sunflower and hazelnut oil, present in adulterated extra virgin olive oil. Furthermore, the present study evaluates the use of such methods to decrease the number of input variables from these otherwise high-dimensional spectra and identify spectral features that may be used to discriminate between different oils.