Identification of various types of edible oils using an Aspectrics' MC2750 EP-NIR Spectrometer

Summary An Aspectrics' MC2750 EP-NIR spectrometer covering the spectral range 1375-2750 nm was successfully employed for the unequivocal identification of three different types of vegetal oils (canola, corn and olive) with no false-positive results. Access to the spectral information in the 2000 - 2600 nm (5000 - 3850 cm-1) range was key to the identification and differentiation of these vegetal oils.

Introduction

An Aspectrics' MC2750 EP-NIR spectrometer was coupled to an external halogen Near IR source and a 2mm. process transmission fiber probe in order to test the device's ability to positively identify and differentiate samples of canola, corn and olive oils with no false-positive results.

The use of a multivariate chemometrics approach on the second order derivative Near IR spectra of all samples proved unequivocally that each type of oil could be identified (4 independent repeats were done), and that the model was solid enough to prevent even partial false-positive results.

Access to the spectral information in the 2000 - 2600 nm (5000 - 3850 cm-1) range was key to the identification and differentiation of these vegetal oils.

Experiment

Samples:

- Commercially available samples of canola, corn and olive oils were used for this experiment

Apparatus:

- Aspectrics MC2750 EP-NIR spectrometer covering the 1375-2750 nm range
- External halogen Near IR source
- Process transmission fiber probe (600 microns polyimide) with 2 mm. pathlength

Data Collection:

- All spectra were collected using Aspectrics' RTSS Chemometrics software package. A 30-second time parameter was used for data collection. All samples were analyzed in 4 identical test conditions, repeating a new background between each assay.
- Data treatment consisted of:
  - calculating absorbance spectra from a single beam intensity spectra using an open beam configuration as a background;
  - calculating the second order derivative for each absorbance spectrum; and,
  - developing Principal Component Analysis (PCA) based methods for the identification of each type of oil.

Results & Discussion

Initial chemometrics testing was conducted on the absorbance spectra (Figure 1). This approach yielded no significant result as the Near IR spectroscopic differences in the three types of oils were too small to be identified and modeled using a PCA approach.

However, when these very small variations were enhanced by calculating the second order derivative spectrum of each of the sample absorbance, spectral regions ranging from 1600 – 1950 nm and 2000 – 2600 nm (Figures 2, 3 and 4), these three materials were readily identified.

Figures 5, 6 and 7 illustrate the method's ability to clearly identify and differentiate each type of oil. It is observed that:

- when projecting the EP-NIR spectrometer response in a space designed to identify corn oil, not only are all 4 corn oil spectra plotted within the 99% probability space of "100% probability of being corn oil", but also that the remaining 8 samples (canola and olive oils) are plotted within the 99% probability space of "0% probability of being corn oil" (Figure 5).
- when projecting the EP-NIR spectrometer response in a space designed to identify canola oil, not only are all 4 canola oil spectra plotted within the 99% probability space of "100% probability of being canola oil", but also that the remaining 8 samples (corn and olive oils) are plotted within the 99% probability space of "0% probability of being canola oil" (Figure 6).
- when projecting the EP-NIR spectrometer response in a space designed to identify olive oil, not only are all 4 olive oil spectra plotted within the 99% probability space of "100% probability of being olive oil", but also that the remaining 8 samples (canola and corn oils) are plotted within the 99% probability space of "0% probability of being olive oil" (Figure 7).

Conclusion

This experiment proves conclusively that an Aspectrics' MC2750 EP-NIR spectrometer can identify and differentiate chemically similar edible oils in various mixtures.

Furthermore, the 2000-2600 nm spectral region was key to differentiating the various oils.

Aspectrics

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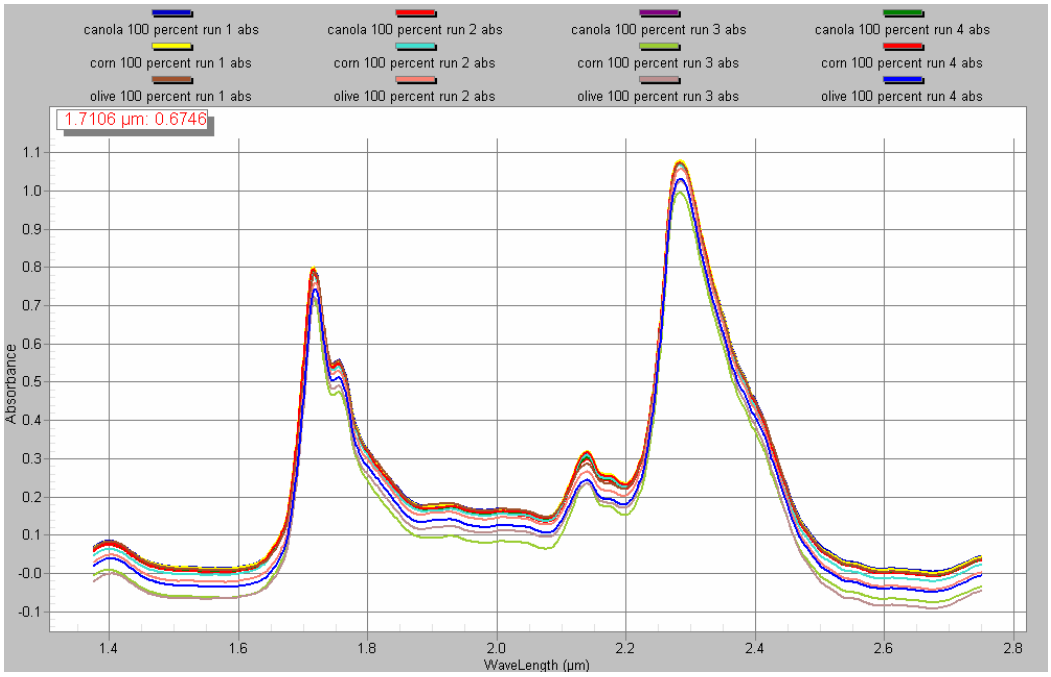

Figure 1:

EP-NIR spectra of canola, corn and olive oils (4 repeats for each sample).

Data collected in 30 seconds using a process transmission fiber probe (600 microns polyimide) with 2 mm. path length

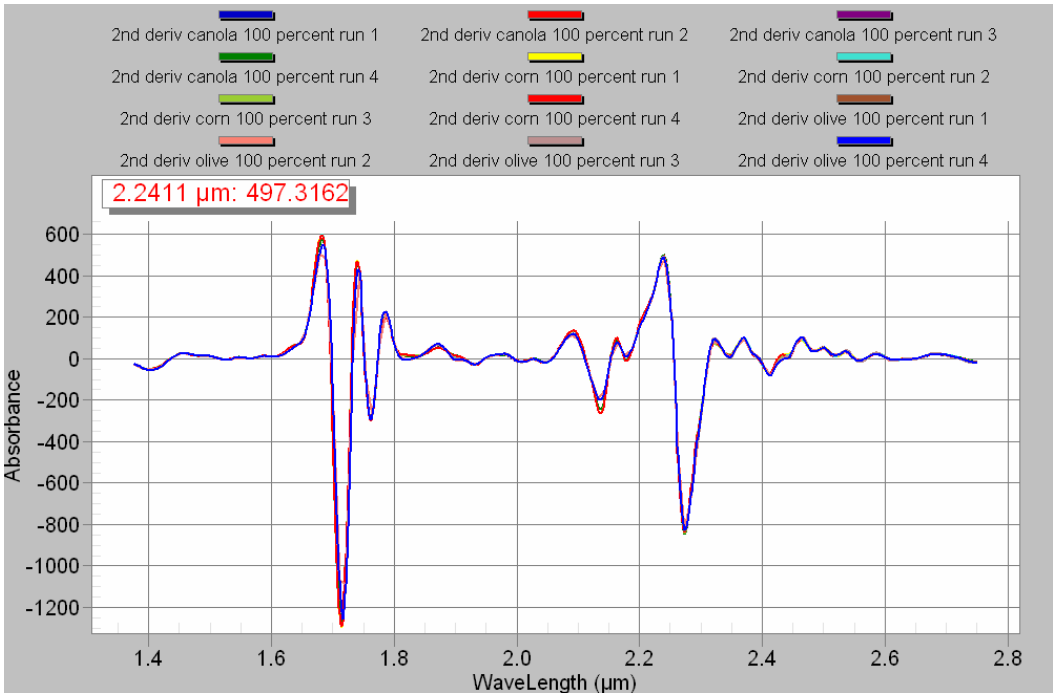

Figure 2:

Second derivative EP-NIR spectra of canola, corn and olive oils (4 repeats for each sample).

Data collected in 30 seconds using a process transmission fiber probe (600 microns polyimide) with 2 mm. path length

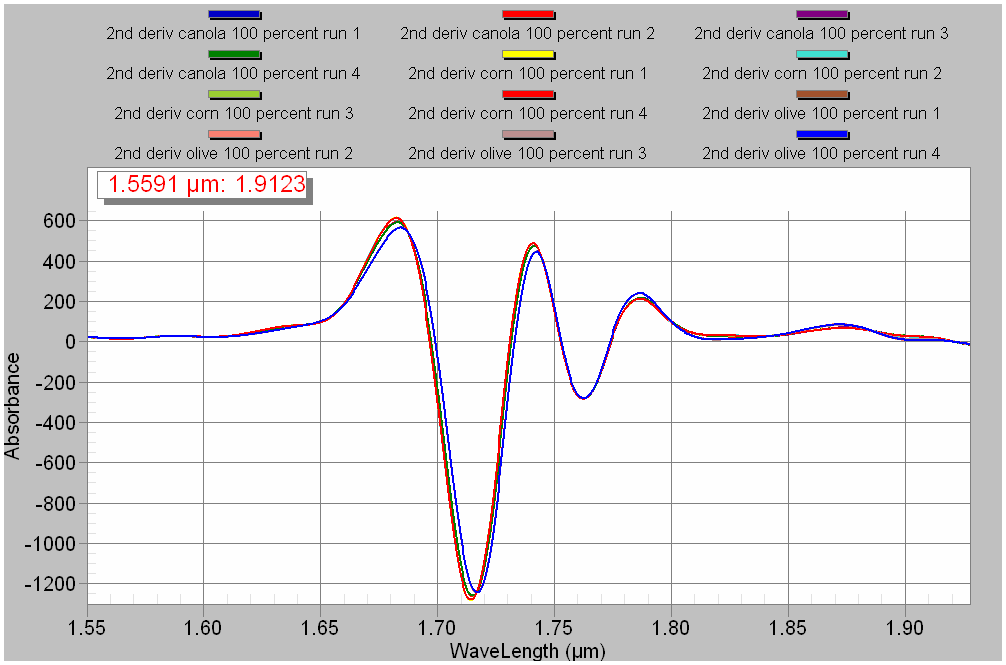

Figure 3:

Second order derivative of EP-NIR spectra of canola, corn and olive oils (4 repeats for each sample), zoomed in on region 1600-1950 nm.

Data collected in 30 seconds using a process transmission multimode fiber probe (600 microns polyimide) with 2 mm. path length

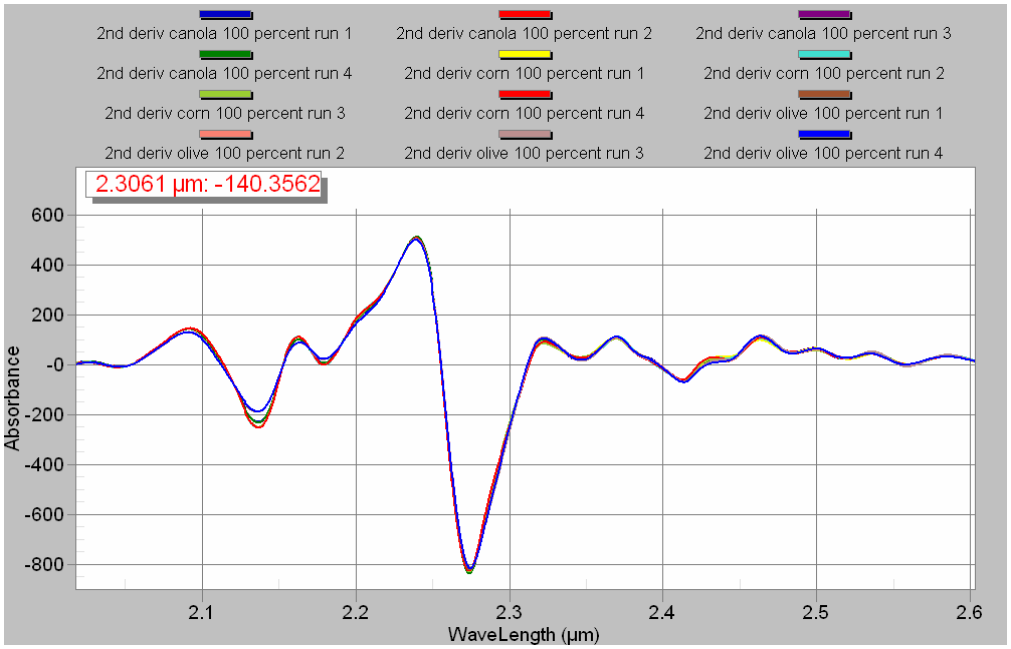

Figure 4:

Second order derivative of EP-NIR spectra of canola, corn and olive oils (4 repeats for each sample), zoomed in on region 2000-2600 nm.

Data collected in 30 seconds using a process transmission multimode fiber probe (600 microns polyimide) with 2 mm. path length

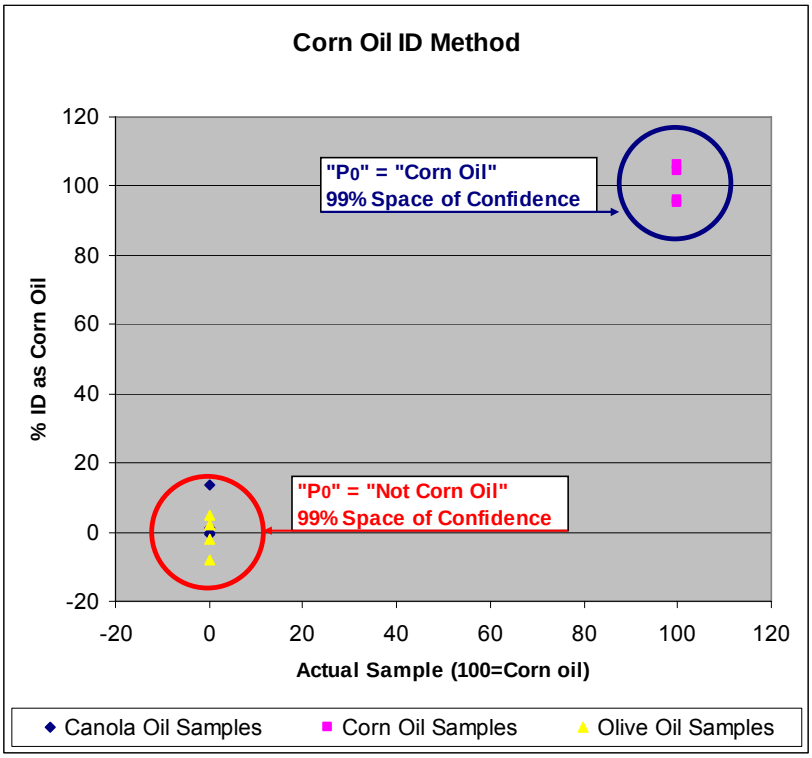

Figure 5:

Identification of corn oil samples

The ***blue circle*** designates the 99% space of confidence for positive identification of **corn** oil samples. All spectra for repeated measurement of corn oil samples are well with the space of confidence for a positive identification as corn oil.

The ***red circle*** designates the 99% space of confidence for positive identification of **not corn oil** samples.

All other spectra are well within the space of confidence as not being corn oil samples.

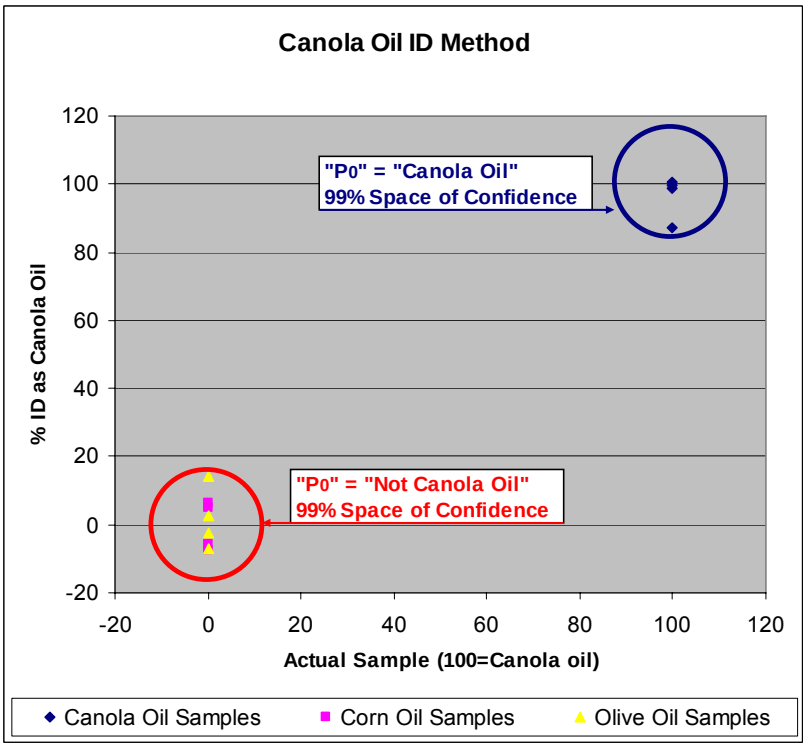

Figure 6:

Identification of canola oil samples

The ***blue circle*** designates the 99% space of confidence for positive identification of **canola** oil samples. All spectra for repeated measurement of canola oil samples are well with the space of confidence for a positive identification as canola oil.

The ***red circle*** designates the 99% space of confidence for positive identification of **not canola oil** samples.

All other spectra are well within the space of confidence as not being canola oil samples.

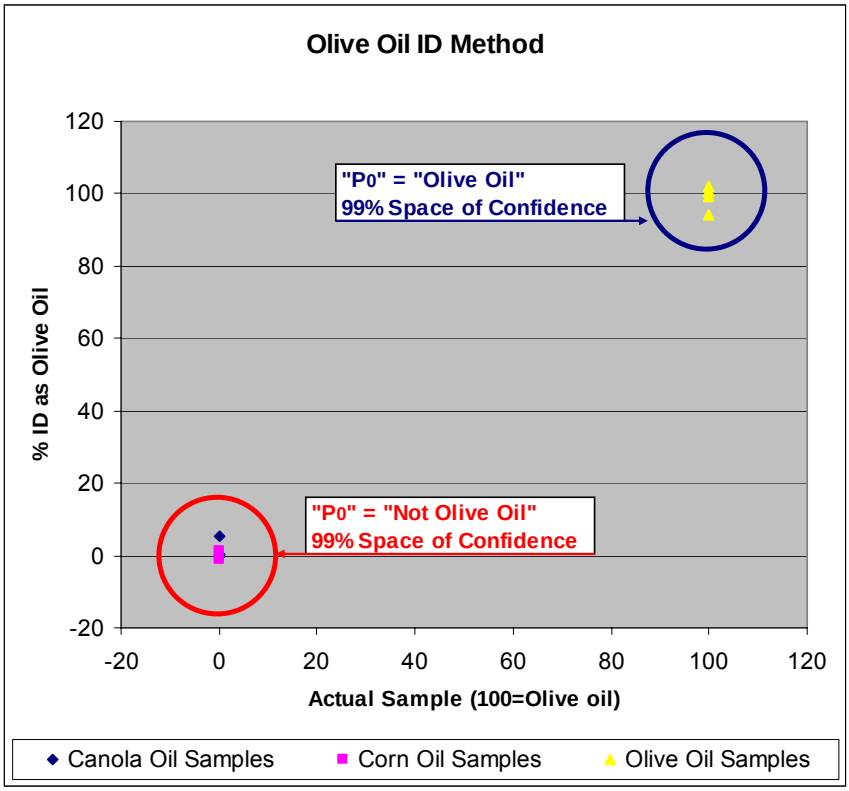

Figure 7:

Identification of olive oil samples

The ***blue circle*** designates the 99% space of confidence for positive identification of **olive** oil samples.
All spectra for repeated measurement of olive oil samples are well with the space of confidence for a positive identification as olive oil.

The ***red circle*** designates the 99% space of confidence for positive identification of **not olive oil** samples.

All other spectra are well within the space of confidence as not being olive oil samples.

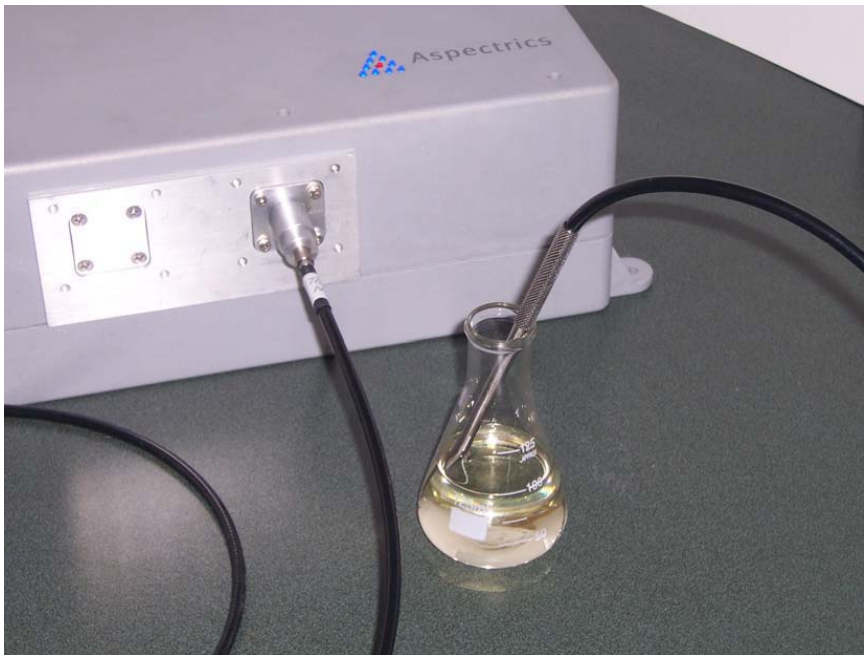

Figure 8:

Aspectrics' MC2750 EP-NIR spectrometer with a process transmission multimode fiber probe (600 microns polyimide) with 2 mm. path length