

The rapid characterization of natural products and herbal medicines by near-infrared spectroscopy

MARIKO KUDO, ANTHONY C. MOFFAT AND ROBERT A. WATT

Centre for Pharmaceutical Analysis, The School of Pharmacy, University of London, 29-39 Brunswick Square, London WC1N 1AX

Near-Infrared Spectroscopy (NIRS) in the 800-2500 nm region can provide simultaneous information about the chemical composition and physical state of materials including moisture content and particle size data (Moffat *et al.* 1997). Spectroscopy in this region has been slow to be exploited as complex, computer-based statistical analysis (chemometrics) is necessary to complete analysis of the information rich spectra. Although the technique has been extensively used in the agriculture and food industry, there has been only one early use for the differentiation of extracted herbal medicines (Corti *et al.* 1990).

Here we demonstrate the potential of NIRS for the analysis of crude and prepared natural products in order to achieve identification, confirm purity and check for adulteration. The technique is rapid, non-destructive and complementary to traditional analytical methods. Samples of *Umbelliferae* fruit have been examined as a number of members of the family are in use and as the fruits can be superficially similar, problems arise due to misidentification and adulteration with great differences in active content between varieties and with the presence of toxins in some members of the family.

Samples of *Umbelliferae* fruit in the dried state were scanned on a FOSS NIRSystems 6500 Rapid Content Analyser in 10mm glass vials in diffuse reflectance mode. In the first instance, identification was completed using FOSS Vision software by a wavelength distance statistical comparison method on Standard Normal Variate corrected and 2nd derivative transformed spectra (Fig. 1.). Twelve sample spectra, each of 32 scans, were obtained for each sample.

By this method, six samples of fennelseed (*Foeniculum vulgare*) could be completely identified as distinct from seven of hemlock (*Conium maculatum*) even though each set contained examples of different ages and varieties. All samples were presented as the unprepared crude seed material.

Similar complete identification of the two *Umbelliferae* sets was achieved when the samples were presented in the ground state.

Examination of a library of spectra of eleven fennelseed samples, five hemlock, two aniseed, two caraway, two coriander, and three dill archive samples allowed the complete identification of each type in both the crude and ground states.

This is of particular interest as hemlock (*Conium maculatum*) contains the toxic alkaloid coniine and is known to potentially adulterate anise fruits.

While the differentiation of ground from unground samples can also be achieved using NIRS, we are continuing to develop techniques to make sample identification independent of the form of the sample, and hence much more general. The identification of varieties, age of sample, determination of moisture content and purity is also currently under investigation.

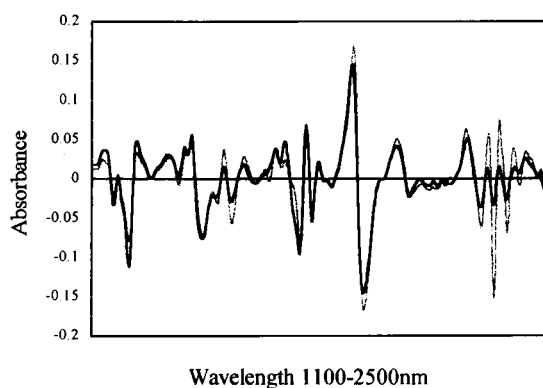


Fig. 1. Second derivative SNV-transformed spectra of a sample of fennel (dark trace) and hemlock (light trace)

The authors thank FOSS NIRSystems for the loan of a spectrometer and Mrs. Sheelagh Halsey for advice. We thank Mr. Martin Domin and Mr. Charlie Smith of Myddleton House gardens for seed samples.

References

- Moffat, A.C., Jee, R.D., Watt, R.A. (1997) New Near-Infrared Centre of Excellence for Europe, *Eur. Pharm. Rev.* 2: 37-40
- Corti, P., Dreassi, E., Franchi, G.G., Corbini, G., Moggi, A., Gravina, S. (1990) Application of NIR Reflectance Spectroscopy to the Identification of Drugs Derived from Plants. *Int. J. Crude Drug Res.* 28: 185-92