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RAPID ASSESSMENT OF FOOD ADULTERATION USING PYROLYSIS MASS SPECTROMETRY AND NEURAL NETWORKS

by

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There is a continuing requirement for methods that might be exploited for the rapid characterisation of biological systems, for instance in determining whether a particular foodstuff is what it claims to be, or whether it has been adulterated with or substituted by a lower-grade material.

A novel approach to the solution of this problem has been developed by combining two techniques - pyrolysis mass spectrometry and artificial neural networks. It is illustrated here by its application to the distinction between extra virgin and adulterated olive oils.

Virgin olive oil is the oil extracted by purely mechanical means from sound, ripe fruits of the olive tree. Such oils with a free fatty acid content (in terms of oleic acid) below 1% are known as "extra virgin", while oils with good flavour but greater acidity may be graded as "fine" or "semi-fine". Lower grades, including those that have been subjected to refining, may be known as "lampante" or "pure".

Olive oil is considered to contribute significantly to the nutritional and health benefits of Mediterranean-type diets and, uniquely among vegetable oils, its flavour is best enjoyed without refining. Olive oil therefore commands a higher price mean there is a great temptation to adulterate olive oils with other seed oils.

Pyrolysis Mass Spectrometry

A number of methods have been proposed for the detection of olive oil adulteration, for example chromatographic, near infrared and UV spectrophotometric methods, though none appears to have found widespread usage.

Pyrolysis is the thermal degradation of complex material in an inert atmosphere or a vacuum. It causes molecules to split at their weakest points to produce smaller, volatile fragments called pyrolysate. A mass spectrometer can then be used to separate the components of the pyrolysate on the basis of their mass-to-charge ratio (m/z), so as to produce a pyrolysis mass spectrum. This can then be used as a "chemical profile" or fingerprint of the complex material analysed. The overall technique is known as pyrolysis mass spectrometry (PyMS).

Chemometrics is the discipline concerned with the application of statistical and mathematical methods to chemical data. A related approach is the use of (artificial) neural networks (ANNs). These can be considered as collections of very simple "computational units", which can take a numerical input (pyrolysis mass spectra) and transform it into an output (that is, determine whether oil is of virgin quality or adulterated).

The great power of neural networks stems from the fact that it is possible to "train" them. When training is completed, the ANN may then be exposed to "unknown" pyrolysis mass spectra and will then "immediately" output the status of the oils. If the outputs from the previously unknown inputs are accurate, the trained ANN is said to have "generalised".

Experiment Protocol

For the olive oil experiment, two sets of samples were prepared, each consisting of 12 samples of various extra virgin olive oils, plus 12 samples variously adulterated with 5-50% of soya, sunflower, peanut, corn or rectified olive oils. The experiment was performed double-blind, such that the identities of the second set were not known. PyMS was performed at 530°C using a Horizon Instruments machine.

ANN analyses were carried out with a user-friendly neural network simulation program, NeuralDesk, which runs under Microsoft Windows/3.1 on an IBM-compatible PC. To ensure maximum speed, an accelerator board was used for the PC (NeuSprint), based on the AT&T DSP32C chip and obtained from the same source, which effects a speed enhancement of some 100-fold, permitting the analysis (and updating) of some 400 000 weights per second.

An ANN was trained consisting of an input layer of the 150 normalised averaged ion intensities from the pyrolysis mass spectra of the first set of oils with mass range 51-200, and one hidden layer of 8 nodes, using the standard back-propagation algorithm, coding virgin oils as 1, non-virgins as 0. The effectiveness of training was expressed in terms of the root mean squared (RMS) error between the actual and desired outputs over the entire training set.

When training had ceased (that is, when an RMS error of 0.001 had been attained), the trained ANN was interrogated with the normalised averaged ion intensities of the pyrolysis mass spectra from the second set of oils (the unknowns). When the code was broken, it transpired that the ANN had correctly assessed each oil. In a typical run, the virgins were assessed with a code of 0.99976 ± 0.000146 (range 0.99954 - 1.00016) and the non-virgins with a code of 0.001079 ± 0.002838 (range 0.00026 - 0.01009).

Discriminating Power

PyMS has major advantages of speed (the typical sample time is less than two minutes) and automation, which allow approximately 300 samples to be analysed daily. Furthermore, after the initial outlay of some £50 000 on the British-made system, running costs are relatively cheap, typically about £1 per sample.

The discriminating power of the approach is enormous, since if each (normalised) mass is accurate to within 10% there are 10^{150} possible pyrolysis mass spectra, and all biological material may be pyrolysed in the way described.

The study reported here (and supported by the United Kingdom Science and Engineering Research Council) clearly shows that the use of pyrolysis mass spectrometry and artificial neural networks was able rapidly and accurately to assess the contamination of virgin olive oils with 5-50% corn, peanut, soya, sunflower oil, or rectified olive oil.

In conclusion, the combination of these two techniques constitutes a novel, powerful and universal approach to the assessment of food adulteration. (110293/RS)

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CAPTION FOR ILLUSTRATION ACCOMPANYING
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Caption No TG 463/2/1	The Horizon Instruments pyrolysis mass spectrometer.