ANALYTICAL METHODS

NPARR 3(1), 2012-0114, **Classification of olive oils according to geographical origin by using ^{1}H NMR fingerprinting combined with multivariate analysis**

Authentic extravirgin olive oils from 7 different regions (Italy – 3 regions, Greece – 4 regions) have been investigated by ^{1}H Nuclear Magnetic Resonance (NMR) fingerprinting in combination with multivariate statistical analysis. In order to cover the dominating lipid signals as well as signals from compounds of low abundance in the oil, both a simple one pulse experiment and an experiment with multiple saturation of the lipid signals was applied to each sample. Thus, the dynamic range of concentrations covered by the two experiments was of the order of 100,000 allowing for a more comprehensive NMR assessment of the samples. Monte-Carlo embedded cross-validation was used to demonstrate that a combination of principal component analysis, canonical analysis, and classification via nearest class mean can be used to predict the origin of olive oil samples from ^{1}H NMR data. Given the rather limited number of samples tested, correct prediction probabilities of 78% were achieved with region specific correct predictions between 53% and 100% [F. Longobardi, A. Ventrella, C. Napoli, E. Humpfer, B. Schütz, H. Schäfer, M.G. Kontominas and, A. Sacco* (Dipartimento di Chimica, Università degli Studi di Bari "Aldo Moro", Via Orabona 4, 70126 Bari, Italy), *Food Chemistry*, 2012, **130**(1), 177-183].

NPARR 3(1), 2012-0115, **Microwave-assisted extraction of chlorogenic acids from green coffee beans**

Microwave-assisted extraction (MAE) has been considered as a potential alternative to conventional solvent extraction for the isolation of phenolic compounds from plants. Aqueous and alcoholic extracts of green coffee bean obtained by MAE were quantitatively analysed for total yield of extracts, chlorogenic acids, caffeine and total polyphenol content. The extracts were also evaluated for radical-scavenging activity, using 1, 1-diphenyl-β-picrylhydrazyl radical. Under optimum conditions of time (5 min), temperature (50°C) and wattage (800 W), the maximum chlorogenic acids and caffeine could be extracted with water as solvent. The extracts contained chlorogenic acids and caffeine in the ranges of 31-62% and 22-40%, respectively. The yields of MAE under optimum conditions were higher than those from the conventional solvent extraction at 5 min and 50 °C and the extracts showed radical-scavenging activity of >75%, even at the concentration of 25 ppm. The MAE process can thus be predicted and controlled for industrial application [Rohit Upadhyay, K. Ramalakshmi, L. Jagan Mohan Rao*(Plantation Products, Spices and Flavour Technology Department, Central Food Technological Research Institute (Council of Scientific and Industrial Research), Mysore 570 020, India), *Food Chemistry*, 2012, **130**(1), 184-188].

NPARR 3(1), 2012-0116, **Chemometric approach to evaluate trace metal concentrations in some spices and herbs**

Herbs (mint, thyme and rosemary) and spices (black pepper, chili pepper, cinnamon, cumin, sweet red pepper and turmeric) were analysed using atomic spectrometry and then subjected to chemometric evaluation in an attempt to classify them using their trace metallic analyte concentrations (As, Ba, Ca, Cd, Co, Cr, Cu, Fe, Mg, Mn, Ni, Sr and Zn). Trace metals in acid digests of these materials were determined using both inductively coupled plasma-atomic emission spectrometry and inductively coupled plasma-mass spectrometry. The chemometric techniques of principal component analysis (PCA), linear discriminant analysis (LDA) and cluster analysis (CA) were used for the classification studies. These herbs and spices were classified into five groups by PCA and CA. When the results of these techniques were compared with those from LDA, it was found that all group members determined by PCA and CA are in the predicted group that 100.0% of original grouped cases correctly classified by LDA [Cennet Karadaş and Derya Kara* (Department of Chemistry, Art and Science Faculty, Balikesir University, 10100 Balikesir, Turkey), *Food Chemistry,* 2012, **130**(1), 196-202].

NPARR 3(1), 2012-0117, **Development and validation of a novel real-time PCR method for the detection of celery (*Apium graveolens*) in food**

The paper presents a novel real-time PCR method allowing the detection of traces of celery (*Apium graveolens*) in complex food matrices. The method is based on the amplification of a sequence of the gene coding for the *Apium graveolens* NADPH-dependent mannose-6-phosphate reductase. It allows the detection of three commonly used celery varieties, celery roots (*Apium graveolens var. rapaceum*), celery stalks (*Apium graveolens* var. *dulce*) and leaf celery (*Apium graveolens var. secalinum*) and does not show any cross-reactivity with 64 biological species, including ten members of the *Apiaceae* family. The limit of detection, determined by analysing serially diluted celery extracts, is 10 pg celery DNA for all three celery varieties. In spiked model sausages, the LOD is 0.005% celery. The real-time PCR method was applied to 26 commercial food products. Celery DNA was found in one out of ten samples without any information about the presence of celery [Magdalena Fuchs, Margit Cichna-Markl* and Rupert Hochegger (Department of Analytical Chemistry, University of Vienna, Währinger Straße 38, 1090 Vienna, Austria), *Food Chemistry*, 2012, **130**(1), 189-195]