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Symposium Introduction

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Recent Trends and Advances in Food Chemistry and Analysis: Research Highlights from the IX Italian Congress of Food Chemistry

ABSTRACT: The IX Italian Congress of Food Chemistry (ChimAlSi_2012) contributed 12 lectures, 66 conferences, and 290 posters to the wealth of food knowledge; these were presented in four sessions: food safety, analytical techniques, bioactive compounds, and nutraceuticals. Emerging topics were discussed in two workshops dealing with *food contaminants,* and *food and health*. It has been an excellent forum for passionate exchange of recent results obtained in traditional and emerging fields of food chemistry. The symposium allowed coverage of the broad diversity of food-related topics, comprising food contaminants and food quality and the application of analytical approaches, such as sensorial, physical, chemical, spectroscopic, hyphenated mass spectrometric, biological and chemometric techniques, as well as nutrition and health aspects.

INTRODUCTION

The Italian Congress of Food Chemistry has become established as one of the most renowned Italian international meetings on food chemistry, taking place every 2 years in Italy. The first meeting was held in 1990 in Giardini Naxos, Sicily; since then, this Congress series has become the reference for food scientists as a platform addressing both the width and depth of food science. Participants from academia and industry actively contribute to the symposium and discuss advances and trends in food chemistry in an informal and open atmosphere. Traditionally, many young scientists can present their work, some of them sponsored by the Congress Organizing Committee, and exchange views and experiences with well-known experts in the area.

The IX Italian Congress of Food Chemistry (ChimAlSi_2012) was organized in Ischia (NA), Italy, in June 2012. About 330 participants contributed 350 lectures and posters to the wealth of food chemistry knowledge. The contributions were grouped in four sessions: food safety, analytical techniques, bioactive compounds, and nutraceuticals. Most of the contributions will be published in the proceedings of the ChimAlSi_2012.[1] In this special issue of the *Journal of Agricultural and Food Chemistry*, only a small number of original works are published, which nevertheless represent well the diversity and trends in Italian food chemistry research.

STATUS AND TRENDS IN FOOD CHEMISTRY

Analytical Methods in Food Safety. The guarantee of food safety and quality along the food chain is a principal demand of consumers. Fundamental aspects in food safety, such as the presence of contaminants and pathogens and their potential risk, are important consumer concerns. To guarantee food safety and quality and satisfy the requirements of the consumer, it is necessary to ensure that efficient analytical methodologies are possessed by the food industry.

New analytical methods are emerging that offer high throughput and easy-handling solutions for industry and control authorities. Complementing traditional methods, these new rapid methods allow on-site testing of food quality and safety.

Two papers discuss the standardization of analytical tools in food safety monitoring. Some geographic regions in southern Europe are more susceptible to contamination with the toxigenic species and ochratoxin A (OTA). Longobardi et al.[2] report the development of a new analytical method for the determination of OTA in Primitivo red wine, using immunoaffinity and aminopropyl solid-phase column cleanup and spectrofluorometric measurement after spectral deconvolution, with reduction of cost and time of analysis when compared with AOAC Official Method 2001.01.[3] OTA was first detected as a wine contaminant in 1996, and the role of *Aspergillus* section *Nigri* and *Aspergillus carbonarius* in OTA production was discovered in Europe in 1999, and a novel approach for the rapid analysis of OTA in wine samples using dispersive liquid−liquid microextraction (DLLME) was reported recently.[4]

Among the foodstuffs, milk and cheese are often subject to adulterations because of their economical and nutritional values. Depending on the local laws of the country, the most common practices concerning these products are milk dilution by whey or water, mixing of different milk species, and addition of milk anhydrous products (caseins and caseinate, milk protein concentrate, whey proteins, powdered milk) to liquid milk. Among the analytical methods employed for milk adulteration investigation, the most used are HPLC and GC for quantitative determination of furosine produced from the acid hydrolysis of lactosylated proteins. Few studies have been dedicated to the detection of milk adulteration considering the protein modifications occurring after thermal processes in powder milk. Calvano et al.[5] analyze the tryptic digests relevant to samples of commercial cow's milk, raw cow's milk, and powdered cow's milk, and some diagnostic peptides of powdered milk, attributed to modified proteins, were identified.

Analytical Methods in Food Quality. European wine production represents about 70% of world production, and thus it is an important export commodity. During aging in the bottle of red wines, changes in phenolic composition occur and the chemical transformations involved depend on the oxygen intake of wines. These changes are responsible for color stabilization and astringency decrease of red wine. Astringency is a tactile sensation that derives from the interaction between salivary proteins and wine tannins, resulting in their complexation and subsequent precipitation in the oral cavity. Gambuti et al.[6]

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evaluate the effect of oxygen exposure of red wine, before (micro-oxygenation) and after (nano-oxygenation) bottling, on the phenolic composition and astringency of wine. The astringency was evaluated by sensory analysis and by a method based on the SDS-PAGE electrophoresis of salivary proteins after reaction of saliva with wine (saliva precipitation index, SPI). Micro-oxygenation caused a decrease of wine astringency and a stabilization of color.

Caretti et al.[7] develop a novel and efficient analytical method to define the fat-soluble vitamin and carotenoid profile of milk from different animal species. Overnight cold saponification was optimized as a simultaneous extraction procedure, and the whole analytical approach was devised to perform both quantitative and qualitative analyses within the same chromatographic run. Analytes were separated by nonaqueous reversed-phase chromatography and detected by diode array detector and positive atmospheric pressure chemical ionization mass spectrometry. Twelve compounds (*all-trans*-lutein, *all-trans*-zeaxanthin, *all-trans*-β-cryptoxanthin, *all-trans*-β-carotene, retinol, α-, γ-, and δ-tocopherols, ergocalciferol, cholecalciferol, phylloquinone, and menaquinone-4) were quantified in selected reaction monitoring scan mode.

Gluten proteins are responsible for the functional characteristics of wheat flour. A series of investigations showed that high molecular weight glutenin subunits (HMW-GS) are closely associated with the breadmaking quality of wheat flour, especially dough viscoelasticity. The analysis of HMW-GS is hindered by several difficulties because of the complexity resulting from the presence of sequence repeating motifs. This last event produces a number of protein isoforms differing in length by only a few amino acid residues. Mass spectrometry techniques have in part contributed to the assessment of HMW-GS heterogeneity. Ferranti et al.[8] report the analysis of glutenin extracted from several Italian durum wheat cultivars by LC-ESI-Q/TOF. This strategy can be used for the rapid identification and screening of desirable HMW-GS associated with superior quality in wheat breeding programs.

Sample Preparation Methods. The sample preparation procedure consists if converting a real matrix into a sample in a format that is suitable for analysis by a separation or other analytical technique. Although many traditional sample preparation methods are still used, the goals of modern techniques are the ability to use smaller initial sample sizes even for trace analysis, greater specificity or greater selectivity in extraction, increase of automation or reduction of manual operations, and finally a more environmentally friendly approach with less waste and use of small volumes or no organic solvents. Thus, a wide range of modern techniques have been developed having common purposes: to remove the potential interferents from the sample, increasing the selectivity of the method; to increase the concentration of the analyte and, hence, the sensitivity of the assay; to convert the analyte into a more suitable form for detection and separation; and to provide a reproducible method that is independent of variations in the sample matrix.

Highly sensitive techniques such as LC-MS/MS and GC-MS/MS, traditionally used to perform qualitative and accurate quantitative analysis of foodstuff samples, require time- and chemical-consuming steps for sample preparation prior to the instrumental analysis step. Recently, a number of different ambient ionization methods such as direct analysis in real time (DART) or desorption electrospray ionization (DESI) have been introduced to address the problem of MS analysis of untreated samples in their native state, that is, without prior sample preparation or chromatographic separation, and many papers presented in the form of oral communication at ChimAlSi_2012 congress were focused on these issues.[1]

Solid-phase extraction is a widely used sorbent technique that involves the use of disposable cartridges to trap analytes and separate them from the bulk of the matrix. Molecularly imprinted polymers (MIPs) are functional polymers generated by molecular imprinting, an efficient method for producing functional materials equipped with selective identification characteristics. The technique consists of self-assembly of a functional monomer and a template molecule in solution followed by copolymerization of the functional monomer with an excess of an appropriate cross-linking monomer. After removal of the template, the resulting polymer exhibits high affinity for the molecule used as template and structural analogues. In recent years the derived molecularly imprinted solid-phase extraction (MISPE) cartridges have been successfully applied to solve several challenging issues in food, biological, and environmental analysis. Euterpio et al.[9] report the determination of phenolic compounds in food matrices using a MIP as sorbent material in a MISPE. Components of propolis and olive oil, as well as other food matrices, have been of considerable interest in recent years because of their potential utility as pharmaceutical agents for their antioxidant and anticarcinogenic activity.

Enzyme-assisted aqueous extraction processing (EAEP) is an increasingly viable alternative to hexane extraction of soybean oil. Although considered to be an environmentally friendly technology whereby edible oil and protein can be simultaneously recovered, this process employs much water and produces a significant amount of protein-rich aqueous effluent (skim). Cuccolini et al.[10] investigate the possibility of extracting lycopene from tomato waste peels using a green chemistry protocol devoid of organic solvent and with an enzymatic mixture of cellulose and pectinase at 50 °C and pH 5. Further improvement in lycopene concentration is obtained by a second enzymatic treatment with a protease cocktail at 50−60 °C at basic pH for 3 h. This catalytic step eliminates unwanted proteins that are bound to the chromoplasts, but are not essential for their stability, by hydrolyzing the peptide bonds. The final product shows a lycopene content of about 8−10% (w/w, dry basis), which represents a 30-fold increase with respect to the lycopene concentration of the untreated peels.

Flavor and Sensorial Analysis. The flavor quality of a roasted food depends on the roasting process to which it has been submitted. Correct conditions for industrial roasting process are in general obtained from a suitable scaling-up of the results of experiments carried out in pilot or laboratory plants monitored by online easy and fast control methods. Liberto et al.[11] describe a nonseparative headspace−solid-phase microextraction−mass spectrometry (HS-SPME-MS) approach in view of its application to online monitoring of a roasting process. HS-SPME is a high concentration capacity technique characterized by high and reliable recovery, it is easy to automate and to directly online combine with mass spectrometry (MS-nose or mass sensor). The resulting system can give quick representative and diagnostic fingerprints of the volatile fraction of samples in a set and, in combination with a suitable chemiometric analysis, can successfully be applied to characterize, differentiate, or discriminate them. The experimental HS-SPME-qMS results in the monitoring of coffee and hazelnut roasting process are reported and critically discussed.

The application of advanced analytical techniques in the control of the chiral nature of food ingredients may be used to detect adulterations and especially the authenticity of fragrances. Schipilliti et al.[12] study numerous samples of different citrus essential oils by enantioselective-multidimensional gas chromatography (Es-MDGC) and gas chromatography−combustion−interfaced isotope ratio−mass spectrometry (GC-C-IRMS) to determine if the combination of enantiomeric ratios with the carbon isotope ratios can be effective in determining the genuineness of the samples studied.

From Biosensors to the Electronic Nose. For ages, there has been much interest in the design of devices for the sensing of food flavor. The devices, or instruments, are claimed to operate on principles similar, in many aspects, to the human olfactory system. Today, the methodologies devoted to the sensory assessment of foodstuffs are based on either the classical panels of trained human beings or the analysis of some chemical compounds by headspace−gas chromatography−mass spectrometry or the global evaluation of the odor intensity of volatile compounds by the emergent sensor technologies. Recent advances in sensor devices have allowed the development of new applications in many technological fields. Enzyme biosensors are a good alternative thanks to their inherent robustness, selectivity, and sensitivity and the low cost of equipment and ease of sample preparation. Biosensors are successfully applied to the control of ethanol, lactate, glutamate, and pesticide content in wine, milk, and fruit juice, and many papers presented at the Congress described the application of electrochemical disposable biosensors in food analysis.[1]

The name "electronic nose" (e-nose) is due to the similarities between this instrument and the physiological system. There are many applications related to toxic gases, the environment, and medicine. However, the main applications are found in food industry. The applications in foodstuffs include quality assessment, control of the manufacturing process, checking the aroma, changes during storage, and study of packaging materials. Rizzolo et al.[13] explain the relationships between electronic nose pattern, maturity of peaches at harvest time measured by time-resolved reflectance spectroscopy (TRS), and quality evolution during a 4 week cold storage. Peaches and nectarines quickly ripen at ambient temperature, and cold storage is used to slow both the ripening process and decay development. Peaches, cultivar 'Spring Belle', were divided into three TRS maturity classes and randomized into nine samples of 30 fruit each. Peaches of each sample were analyzed for ethylene production by GC, aroma pattern by electonic nose and static HS-GC, sugar (glucose, fructose, sucrose, sorbitol), and organic acid (quinic, malic, citric acids) compositions by HPLC. Data were analyzed by PCA statistical analysis.

Recently a new generation of e-nose systems, based on mass fingerprinting and considered to be more compatible with the basic knowledge of aroma chemists concerning the complexity and specificity of odor perception and the relation with food flavor, was introduced.

Bioactive Compounds. Bioactive compounds in foods have been the topic of many papers over the past 20 years and are among those that have received a higher citation in agricultural and food science journals. Functional foods that contain significant amounts of bioactive components may provide desirable health benefits beyond basic nutrition and play important roles in the prevention of chronic diseases. In particular, regular consumption of fruits and vegetables is associated with reduced risks of cancer, cardiovascular disease, stroke, Alzheimer's disease, cataracts, and some of the functional declines associated with aging. Prevention is a more effective strategy than is treatment of chronic diseases. Therefore, it is very useful to develop innovative analytical methods able to provide a reliable measurement of the content of these molecules in fruits and vegetables. The *Citrus* genus includes fruits belonging to several species and hybrids commonly used for food and industrial purposes. Mencherini et al.[14] develop an HPLC-PDA-MS method to identify *C*- and *O*-glycosyl flavones, a methoxyflavone, and a series of flavanone *O*-neohesperidosides, commonly present in *Citrus* species. Furthermore, three acylated flavanone dioxalate derivatives of neoeriocitrin, naringin, and neohesperidin, reported previously only in bergamot juice, were identified for the first time in *C. aurantium* from Cuba. An inhibitory effect of the extract on vascular hyperpermeability induced by intradermal injections of phlogistic agents was evaluated in rats.

In addition to being rich in vitamin C, folate, and fiber, some *Citrus* fruits contain auraptene and umbelliferone, coumarin-based molecules that can increase the potential of these fruits as functional foods. Auraptene (7-((*E*)-3,7-dimethylocta-2,6-dienyloxy)-2*H*-chromen-2-one) seems to be promising as an adjuvant for cancer prevention, in particular, against melanoma, gastrointestinal, liver, and mammary cancers. Mercolini et al.[15] develop analytical methods useful to evaluate the content of chemopreventive coumarins in different types of *Citrus*, as well as in the same fruits from several cultivars and at different ripening levels.

A key question is whether a purified phytochemical has the same health benefit as does the whole food or mixture of foods in which the phytochemical is present. Legumes contain a rich variety of phytochemicals, including phytosterols, natural antioxidants, and bioactive molecules such as soyasaponins (SS). Sagratini et al.[16] develop a solid-phase extraction (SPE) coupled to liquid chromatography (LC)−mass spectrometry (MS) method for the quantification soyasaponins I and βg in raw and cooked legumes of difference provenience. The bioaccessibility of SS I and SS βg contained in lentils was determined by using an in vitro digestion model. Legumes are low in fat and rich in proteins, exhibiting a lower glycemic index compared to other starchy foods.

Hydroxytyrosol occupies a prominent position among natural polyphenols because of its antioxidant potency and wide range of biological properties. Several efforts have therefore been directed toward the preparation of hydroxytyrosol derivatives with improved antioxidant and pharmacological activities and different solubility properties, particularly enhanced lipophilicity. Panzella et al.[17] describe the synthesis and evaluation of the antioxidant properties of 5-*S*-lipoylhydroxytyrosol and polysulfide derivatives. All polysulfides were found to have stronger hydrogen donor ability than Trolox in the DPPH assay and acted as efficient hydroxyl radical scavengers at concentration as low as 10 μM in a Fenton reaction inhibition assay. The antioxidant activity was also tested in human hepatocarcinoma cell line (HepG2).

NMR in Food. NMR is recognized as one of the main analytical methodologies for metabolite profiling giving a complete view of the foodstuffs metabolites and, together with a suitable statistical analysis, providing relevant results in terms of foodstuffs quality, geographical origin, processing, raw material, safety, and so on.

Capitani et al. investigate the metabolite profiling of the aqueous extracts of two peach varieties (Percoca and

Flaminia)[18] and of Zespri, CI.GI, and Hayward kiwifruits[19] by means of high-field NMR spectroscopy. Water-soluble metabolites belonging to different classes have been identified. The metabolite profiling together with a suitable statistical analysis was used to characterize and discriminate the varieties.

The wine area is definitely one of those in which NMR has proved most successful in recent years. High-resolution techniques are rather powerful tools for studying minor components of enological products. Classical studies on enological products are normally based on composition data obtained by various analytical techniques; however, because the quality and characteristics of a product are not the simple sum of individual chemical characteristics, NMR analysis with chemometric data analysis certainly is a useful tool in this regard. Papotti et al.[20] use the HR-NMR techniques as molecular fingerprints to serve as indirect indicators of authenticity and quality control of several DOC Lambrusco wines of Modena. The data obtained were coupled with chemometric analysis tools to effectively interpret the complex results collected from the mono- and bidimensional spectra acquired.

In recent years, the use of high magnetic fields and the greater sensitivity and spectroscopic resolution that they bring have stimulated interest in 1D and 2D NMR spectroscopy as a routine method for the analysis of complex mixtures such as honey. Schievano et al.[21] describe the characterization of unifloral honey markers identified through an NMR-based fingerprinting approach.

Malmendal et al.,[22] in a very innovative paper published in *Journal of Agricultural and Food Chemistry*, demonstrate the utility of ^{1}H NMR as a tool to analyze the taste of food without any other chemical analysis. Sensing the odor and flavor of food is a very complex process. It depends not only on the combination of ingredients in the food but also on the taster's emotional state. Trained taste testers eliminate some of the variation, but food processors need more objective ways to measure the sensory descriptor of their products. This is where electronic sensing technologies, such as e-noses, come into play. However, current instruments can analyze only certain food components and require very specific sample preparation. To overcome these shortcomings, Malmendal et al. turned to NMR to test its abilities as "a magnetic tongue". The researchers analyzed 18 canned tomato products from various markets with NMR and found that the instrument could estimate most of the tastes assessed by the human taste testers. The researchers say that the magnetic tongue has good potential as a rapid, sensitive, and relatively inexpensive approach for food-processing companies to use.

CONCLUSION

This special issue of *Journal of Agricultural and Food Chemistry* contains a selection of papers that were presented at the IX Italian Congress of Food Chemistry (ChimAlSi_2012) (Ischia, Italy, June 3−7, 2012). The most promising submissions were proposed for publication in a special issue of *Journal of Agricultural and Food Chemistry* in June 2012. They are original papers on methods in food analysis including physical, chemical, and instrumental methods; several are collaborative works between two or more universities. We thank the contributors who gave so generously of their time and experience and who made this publication a valuable tool for scientists in the field of food chemistry and analysis. We also thank the referees for their valuable comments and for the very detailed and accurate review of manuscripts; their comments certainly helped to improve the papers.

We are also very grateful to the Editorial Board of *Journal of Agricultural and Food Chemistry* for embracing this project with interest and enthusiasm and for the opportunity to publish this special issue. We hope that this will be the first of a long series in this attractive, interesting, and relevant journal. Finally, we thank the Editor-in-Chief, James Seiber, for his valuable input and careful supervision. Thank you Jim.

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