Influence of Thermal Treatments Simulating Cooking Processes on the Polyphenol Content in Virgin Olive Oil

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Contents *(click on the topic)*

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Biofuels and Biobased Products: chemistry of biofuel and biobased products, including feedstocks, conversion, refining, waste utilization, disposal, and sustainability, and environmental emissions and effects associated with these processes.

Chemical Aspects of Biotechnology and Molecular Biology: processes and underlying chemical science involving classical and modern aspects of biotechnology applicable to food and agricultural systems; to include proteomic and genomic techniques applicable to measurement and evaluation in food production and metabolism.

Food and Beverage Chemistry/Biochemistry: chemistry and biochemistry associated with food and beverage production, processing, preparation, composition, packaging and storing, including both naturally occurring and added components.

Food Safety and Toxicology: chemical aspects of toxicology of crop protection, contaminants, and related chemicals and the design and action of chemically related processes that enhance food safety.

Metabolomics Applied to Agriculture and Food (see more details on p 19): applications of metabolomics as related to research topics in agriculture, food, and nutrition, in particular metabolite-targeted analysis and progress in the development of analytical platforms for metabolomics approaches.

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Comments related to published papers will be considered from readers if the correspondence is **received within six months of the date of publication of the original paper**; the authors of the original paper will be given the **opportunity to reply** to such comments within two months, if they so desire. Both comments and replies should not exceed 1000 words each, including citations, and will be published consecutively in the same issue of the *Journal* after peer review. For examples, see *J. Agric. Food Chem.* **2007**, *55*, 7213–7214 and *J. Agric. Food Chem.* **2007**, *55*, 7215–7216; *J. Agric. Food Chem.* **2011**, *59*, 464–465 and *J. Agric. Food Chem.* **2011**, *59*, 466.

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Consult *The ACS Style Guide* and current issues of the *Journal* for examples of reference format.

Authors should cite all prior published work directly pertinent to the manuscript. However, extensive bibliographies that go beyond a direct connection with the manuscript are discouraged. Prior work can often be covered by citation of a few leading references or of review articles. As a general guideline, authors should attempt to limit the literature cited to approximately 50 or fewer citations (except for review or perspective manuscripts).

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References should be cited in the text by superscript numbers, for example, [1,2–5], etc.

Give complete information, using the last name and initials of the author, patentee, or equivalent; do not use “Anonymous”.

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Typical references follow the styles given below.

For journals:

1. Brown, J.; Jones, M.; Green, D. Article title. *J. Agric. Food Chem.* **1980**, *28*, 1–4. (Issue number must be used if each issue of the periodical begins with page 1.)

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2. Smith, L; Caldwell, A. Chapter title. In *Book Title*, edition no.; Keys, F., Park, G., Eds.; Publisher: City, State (or Country if non-U.S.), Year; Vol. no., pp.

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line width	0.6 point (0.021 cm, 0.0084 in.)
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hash spacing	2.5 points (0.088 cm, 0.0347 in.)
as text settings select…	
font	Arial or Helvetica
size	10 points
under preferences choose…	
units	points
tolerances	3 pixels
under page setup choose…	
paper	US Letter
scale	100%

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REPORTING SPECIFIC DATA

Bioactivity. Manuscripts reporting on bioactivity of plant-derived or other extracts must also include identification and characterization of individual chemicals responsible for the observed bioactivity. (See Novel Compound Characterization below.)

For peptide studies, such as anti-ACE peptides, the authors should provide the in vivo animal (or human) data to substantiate activity of the peptides studied and, if no in vivo data are provided, the chemistry must be novel and the amount of work substantial.

Gas Chromatographic Methods. For manuscripts in which gas chromatographic methods are used, see "Reporting of Gas Chromatographic Methods", by Morton Beroza and Irwin Hornstein [*J. Agric. Food Chem.* **1973**, *21*, 7A (located at the back of the January 1973 issue or as a link from the *Journal's* Author Information page)]. Consult recent issues for examples of GC, LC, and other instrument parameter descriptions.

Spectroscopic Data. This is a guide only; in certain cases different methods of data presentation may be more suitable. Authors are encouraged to consult examples of data presentation published in recent issues of the *Journal* for appropriate style and format. **Complete infrared, NMR, mass, or other spectra will be published only if novel or necessary to substantiate points made under the Results or Discussion sections.** Such presentations take up valuable space, and essentially the same information can frequently be put into a much more compact form by simply listing the position and intensity of the maxima. It is usually not necessary to list all of the maxima in the spectra to provide an adequate description. Report the type of instrument used (e.g., in mass spectrometry, whether magnetic, quadrupole, time-of-flight, etc.) and also the type of cell, the solvent (if any), and the state of the sample (whether liquid, gas, solution, etc.).

Mass Spectra. List the molecular ion and about 10 of the major ions with their intensities in parentheses, or more preferably use the method outlined by H. S. Hertz, R. A. Hites, and K. Biemann (*Anal. Chem.* **1971**, *43*, 681–691). This method involves dividing the spectrum into consecutive regions of 14 mass units starting at *m*/*z* 6 (i.e., 6–19, 20–33, 34–47, 48–61, etc.). The two most intense ions in each region are then listed. Intensities, relative to the most intense ion, the intensity of which is taken as 100, are shown in parentheses immediately following the *m*/*z* value; for example: hexanal, mass spectrum found (70 eV, two most intense ions each 14 mass units above *m*/*z* 34): 43 (86), 44 (100), 56 (86), 57 (65), 71 (28), 72 (33), 82 (18), 85 (5), 97 (2), 100 (2). If the molecular ion does not appear in this presentation, the author should indicate it separately.

Nuclear Magnetic Resonance (^{1}H NMR or ^{13}C NMR) Spectra. A document providing detailed information for the presentation of NMR data is now available through "Information for Authors and Reviewers" on the Journal's home page.

The frequency, the solvent, and also the temperature (if other than ambient) used are first specified. The type of unit used (δ or τ) is then stated, followed by the position of the center of gravity of the sharp line, broad line, or spin–spin multiplet in these units. This is then followed by information in parentheses which (1) describes the type of splitting, that is, singlet as s, doublet as d, triplet as t, quadruplet as qd, multiplet as m; (2) gives the value of the number of protons the area represents; (3) gives the coupling constant *J*; and (4) gives the part of the molecule connected with the particular absorption with the protons involved underlined.

An example would be ^{1}H NMR for ethanol (60 MHz, CCl_4): δ 1.22 (t, 3, J = 7 Hz, $CH_2\underline{CH_3}$), 2.58 (s, 1, OH), 3.70 (qd, 2, J = 7 Hz, $OC\underline{H_2}CH_3$).

Other Spectra. In general, list position and intensity of the maxima. In some cases it may be desirable to list points of inflection.

A brief explanation should be given for any abbreviations not in common use.

Examples:

- Reporting liquid chromatography (HPLC) and HPLC/MS: “Analysis of Polyphenolic Antioxidants from the Fruits of Three *Pouteria* Species by Selected Ion Monitoring Liquid Chromatography–Mass Spectrometry”, by Jun Ma et al. *J. Agric. Food Chem.* **2004**, *52*, 5873–5878.
- Reporting data in detail, including UV shifts and IR spectra: “Characterization of Vegetable Oils: Detailed Compositional Fingerprints Derived from Electrospray Ionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry”, by Zhigang Wu et al. *J. Agric. Food Chem*. **2004**, *52*, 5322–5328.

Novel Compound Characterization. For a discussion of the *Journal's* expectations for compound characterization, please read “Compound Identification: A *Journal of Agricultural and Food Chemistry* Perspective” by R. J. Molyneux and P. Schieberle. *J. Agric. Food Chem.* 2007, *55*, 4625–4629 (DOI: 10.1021/jf070242j). It is essential that novel compounds, either synthetic or isolated from natural sources, be characterized rigorously and unequivocally. Supporting data normally include physical form, melting point (if solid), UV/IR spectra if appropriate, ^{1}H and ^{13}C NMR, mass spectrometric data, and optical rotation (when compounds have chiral centers).

Examples:

- Reporting X-ray data: “Racemic and Enantiopure Synthesis and Physicochemical Characterization of the Novel Taste Enhancer *N*-(1-Carboxyethyl)-6-(hydroxymethyl)pyridinium-3-ol Inner Salt”, by Renaud Villard et al. *J. Agric. Food Chem*. **2004**, *51*, 4040–4045.
- Reporting data in detail, including UV shifts: “Novel Flavonol Glycoside, 7-*O*-Methyl Mearnsitrin, from *Sageretia theezans* and Its Antioxidant Effect”, by Shin-Kyo Chung et al. *J. Agric. Food Chem*. **2004**, *52*, 4664–4668.
- Reporting data for previously known compounds: “Phenolic Constituents and Antioxidant Activity of *Wendita calysina* Leaves (Burrito), a Folk Paraguayan Tea”, by Anna Lisa Piccinelli et al. *J. Agric. Food Chem*. **2004**, *52*, 5863–5868.

Flavor Constituents. Manuscripts reporting on flavor constituents should conform to the recommendations made by the International Organization of the Flavor Industry [for details, see the Editorial in the October 1996 issue of *J. Agric. Food Chem*. (*44*, 2941–2941)]. In brief, any identification of a flavoring substance must pass scrutiny of the latest forms of available analytical techniques. **In practice, this means that any particular substance must have its identity confirmed by at least two methods, for example, comparison of chromatographic and spectrometric data (which may include GC, MS, IR, and NMR) with those of an authentic sample.** If only one method has been applied (MS data alone or retention index or Kovats index alone), the identification shall be labeled “tentative”. In addition, authors are encouraged to include at least semiquantitative data on the concentration of an identified component in the original source, for example, foodstuff or plant part. Ranges such as <1 μg/kg, 1–10 μg/kg, and 10–100 μg/kg are acceptable.

Flavor is evoked by smell (aroma) and taste. A good example showing the correct characterization of taste compounds is the study by Czepa and Hofmann (*J. Agric. Food Chem*. **2003**, *51*, 3865–3873). A good example for aroma compound identification is the study by Milo and Grosch (*J. Agric. Food Chem*. **1996**, *48*, 2366–2371).

The use of reference compounds is a must, if data on sensory properties of single compounds are reported. Odor, which is perceived during sniffing of a food extract at a certain retention index,

may be indicative of the presence of a given compound, but not conclusive unless substantiated by chromatographic and/or spectrometric data and comparison with an authentic reference compound.

Soil Classification. Soils used in research should be described down to the family level according to the soil classification scheme given in *Soil Taxonomy, A Basic System of Soil Classification for Making and Interpreting Soil Surveys,* 2nd ed. (Agricultural Handbook 436; U.S. Government Printing Office: Washington, DC, 1999) (available on-line at http://www.nrcs.usda.gov/wps/portal/nrcs/main/soils/survey/class/taxonomy/). Also give series name if known.

This requirement is to allow comparison and extrapolation to other work giving similar soil classifications, as published in journals such as the *Journal of Soil Science*, *Soil Science Society of America Journal*, *Journal of Environmental Quality*, and *Geoderma*. If information is unavailable to classify the soils at the desired family level, classification should be described or estimated at least to the great group level in the same classification system.

Statistics. Manuscripts reporting analytical, biological activity, composition, and related data must include relevant statistical information to support discussion of differences or similarities in data sets. Refer to a standard statistics reference such as *Statistical Methods*, 8th ed.; Snedecor, G. W., Cochran, W. G., Eds.; University Press: Ames, IA, 1989.

Metabolomics. This category considers applications of metabolomics as related to research topics in agriculture, food, and nutrition, in particular metabolite-targeted analysis and progress in the development of analytical platforms for metabolomics approaches. A metabolome is the quantitative set of chemical compounds in a biological system, i.e., a food, at a given time. However, also metabonomics studies, focused on changes in a given metabolome, e.g., induced by environmental conditions or diseases, fall into this category.

Metabolic profiling and metabolomic fingerprinting correlated with multivariate or data-mining methods are acceptable, if presented in a targeted way. For additional information consult "Targeted Metabolomics: A New Section in the *Journal of Agricultural and Food Chemistry*" by J. N. Seiber, R. J. Molyneux, and P. Schieberle, *J. Agric. Food Chem.* **2013**, DOI: 10.1021/jf4046254.

Animal or Human Studies. Manuscripts describing studies in which the use of live animals or human subjects is involved must include under Materials and Methods a statement that such experiments were performed in compliance with the appropriate laws and institutional guidelines, and also name the institutional committee that approved the experiments. For experiments with human subjects, a statement that informed consent was obtained from each individual must be included and the consent forms made available to the *Journal* on request. Reviewers of manuscripts involving animal or human experiments will be asked to comment specifically on the appropriateness and conformity to regulations of such experiments. **Authors are encouraged to note the approval code or number or give the name of the approving office of official.**

Animal Subjects. The use of animals in a study should be employed only when there are no alternative methods for investigating the fundamental questions of the study. In such cases, **it is the ethical responsibility of all authors to ensure that the care of animals is of the highest possible order, that pain and/or distress is minimized, and that the numbers involved are strictly limited** to those essential to fulfill the experimental design. In the United States the care and use of laboratory animals is regulated by the U.S. Department of Agriculture (USDA) under the Animal Welfare Act. Links to the regulations and other information are available at

http://www.aphis.usda.gov/animal_welfare/links.shtml. It is recognized that researchers in other countries may be governed by different laws and regulations. In such cases, experiments should be designed to conform either to the above USDA regulations or to the International Guiding Principles for Biomedical Research Involving Animals (1985), available at http://www.cioms.ch/publications/guidelines/1985_texts_of_guidelines.htm.

Human Subjects. **The use of human subjects in experimental studies requires informed consent.** Such consent requires that the subjects be informed completely not only about the procedures involved but also about the aims, design, and expected outcomes of the study. Consent must be obtained not only when subjects are involved directly in the study but also when samples (tissue, blood, plasma, etc.) are required for in vitro experiments. In the United States the protection of human research subjects is regulated by the U.S. Department of Health and Human Services (HHS). Regulations are available at http://www.hhs.gov/ohrp/. Laws and regulations governing researchers in other countries must be observed, but experiments should be designed to conform to the intent of the HHS regulations as far as possible.

In relation to the subject matter of the *Journal*, experiments involving taste and food quality evaluation and consumer acceptance are exempt from the above regulations [CFR 46.101 (b) (6)]. However, it should be noted that this would not exempt studies in which extracts, isolates, pure compounds, etc., obtained from conventional food sources are subjected to such evaluation.

The *Journal* will reject any manuscript for which there is reason to believe that animals have been subjected to unnecessary pain or distress or when informed consent of human subjects is absent or incomplete.

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