

Scope, Policy, and Instructions for Authors

(Revised January 2008)

SUBMISSION OF MANUSCRIPTS

Manuscripts **must** be submitted via the web using the Paragon Plus Environment (<http://paragonplus.acs.org>). The site's security features limit access to a manuscript to those Editors and reviewers to whom that manuscript is assigned. If coauthors' e-mail and contract information are entered during the submission process, they will be able to track the progress of the manuscript on their own Paragon Plus web pages; however, communications from the editorial offices will be limited to the corresponding author. Authors must also submit revised manuscripts via the ACS Paragon Plus Environment.

E-mailed submissions and hardcopy submissions will not be processed.

All manuscripts **must** be accompanied by a cover letter that includes eight specific points:

1. manuscript title
2. corresponding author's name, address, telephone and fax numbers, and e-mail address
3. if manuscript is not submitted by the corresponding author, submitter's name, address, telephone and fax numbers, and e-mail address
4. e-mail addresses of all coauthors
5. designation of the *Journal's* subject category that best fits the manuscript (see list under Journal Scope in these instructions)
6. **explanation of the manuscript's significance, including its originality, its contribution to new knowledge in the field, and its relevance to research in agricultural and food chemistry**
7. list of graphics the author would like to have published in color
8. **list of at least four recommended reviewers** for the manuscript; include the address, telephone and fax numbers, and e-mail address for each suggested reviewer; do not include reviewers who may have a conflict of interest or are from the authors' department or unit or who are Associate Editors of the *Journal*

Submissions that do not include a cover letter addressing these eight points will not be processed.

Complete instructions for manuscript preparation and a copyright status form are available at the *Journal's* Website and are also printed in the first issue of each volume. Please conform to these instructions when submitting manuscripts.

Authors whose manuscripts are published in the *Journal* will be expected to review manuscripts submitted by other researchers from time to time.

JOURNAL SCOPE

The *Journal of Agricultural and Food Chemistry* publishes complete or full-length fundamental and applied research papers dealing with the chemistry and biochemistry of agriculture and food. The *Journal* also encourages papers with chemistry and/or biochemistry as a major component combined with biological/sensory/nutritional/toxicological evaluation related to agriculture and/or food.

The *Journal* is organized into the following sections:

- Analytical Methods
- Bioactive Constituents
- Biofuels and Bioproducts Chemistry
- Chemical Aspects of Biotechnology/Molecular Biology
- Chemical Aspects of Food Safety
- Chemical Changes Induced by Processing/Storage
- Chemical Composition of Foods/Feeds
- Crop and Animal Protection Chemistry
- Environmental Chemistry
- Flavors and Aromas/Chemosensory Perception
- Food Chemistry/Biochemistry
- Molecular Nutrition
- Toxicology in Agriculture and Food

MANUSCRIPT TYPES

Research articles must report *original research that is expected to have a definable impact on the advancement of science and technology, incorporating a significant component of innovative chemistry*. Originality will be documented by novel experimental results, theoretical treatments, interpretations of data, and absence of prior publications on the same/similar topics.

Expedited Handling. There is no separate Rapid Communications, Notes, or Letters section. However, manuscripts describing results deemed to be highly important and urgent in a field of research will be considered for expedited processing and review. **Only manuscripts reporting complete research, as opposed to preliminary results, will be considered.** A request for expedited handling, along with justification for the request, must be included in the cover letter accompanying the manuscript.

Review articles will be considered that summarize information in a field in which the literature is scattered or treat published data or other information so as to provide a new approach or stimulate further research. Authors considering the preparation of a review **should submit a synopsis to the Editor** to establish whether the manuscript will meet these guidelines.

Perspectives, which explore needs and opportunities in agricultural and food chemistry in a less technical format than a review article, will be considered. Authors should **contact the Editor** to outline the area to be covered before submitting a Perspectives manuscript. For an example, see *J. Agric. Food Chem.* **2007**, *55*, 4281–4288.

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.

Symposia or Topical Collections. The Editor will consider publication of a series of manuscripts reporting or synthesizing original research that are presented in a symposium or otherwise clustered around a single topic. Prospective organizers should **contact the Editor well in advance** to determine whether the subject matter conforms to the *Journal's* goals, criteria, and available space and to obtain specific instructions for submission of the manuscripts. For an example, see *J. Agric. Food Chem.* **2007**, *55*, 3749–3797. Each manuscript will be put through the normal peer-review process.

ETHICS, CONFLICT OF INTEREST

Authors and coauthors are responsible for the integrity of their manuscripts. The Editor may impose a 2 year submission moratorium on authors and coauthors that are found to be in violation of the ethical guidelines.

Authors and coauthors should familiarize themselves by reading the entire *Ethical Guidelines to Publication of Chemical Research*, which are available at the *Journal's* website and are also published in the first issue each year.

Some particularly important points from the ACS Ethical Guidelines are the following:

Multiple Reporting of Research. It is improper for an author to submit manuscripts describing essentially the same research to more than one journal. Resubmission of a manuscript rejected or withdrawn from publication is permissible. Authors are expected to use care when submitting reports of research previously presented at meetings so that double publication does not occur. This applies to figures and tables as well as text. Publication of research in non-English journals constitutes prior publication. (For a discussion of copyright issues related to the use of tables, figures, or text that are published elsewhere, see *The ACS Style Guide*, 3rd ed., Chapter 7.)

Plagiarism. The Editors of this journal will not tolerate plagiarism, including self-plagiarism.

Coauthorship. The submitting author must obtain consent to coauthorship from all coauthors listed prior to submitting the manuscript and include as coauthors all individuals who made significant scientific contributions to the work. Any disagreement between the corresponding author and coauthors after the manuscript is submitted will cause review of the manuscript to cease. (For a discussion of coauthorship, see *The ACS Style Guide*, 3rd ed., Chapter 1.)

Conflict of Interest. Research involving an evaluation of commercial products should not reveal the brand names of such products unless information regarding their manufacture has been made public by the company producing the product. Codes such as letters (A, B, C, etc.) or numbers (1, 2, 3, etc., or I, II, III, etc.) may be used for purposes of identification. If brand names are used, the authors should disclose at the time of submission any financial arrangement they may have with a company whose product figures prominently in the submitted manuscript or with a company making a competing product. An editorial decision will then be made as to whether the manuscript being submitted should be sent out for review. If the paper is deemed to be suitable for review, information concerning any financial arrangement the authors may have with a given company will be held in confidence and will not influence the evaluation of the research and whether the manuscript can be accepted for publication. As a guiding principle, however, it is expected that the authors of such papers should not have any financial interest in a company (or its competitor) that makes a product discussed in the paper. These guidelines do not generally apply to the use of brand names or to the identification of the producers of products that are used for analytical purposes such as instruments, reagents, or kits.

EDITORIAL PEER REVIEW PROCESS

Peer review is used to help ensure the **highest possible quality** in published manuscripts. For a discussion of this, see "The Importance of Peer Review" by H. L. Wheeler and W. B. Wheeler, *J. Agric. Food Chem.* (Editorial) **2006**, *54*, 8983–8983. Scientists with expertise in the subject matter being treated will evaluate the manuscript for validity of the experimental design and results, originality, significance, and

appropriateness to the *Journal*. **The Editors may exercise their prerogative to decline a manuscript without peer review if that paper is judged to be outside the scope of the *Journal* (lacks significant chemistry/biochemistry), poorly written or formatted, fragmentary and marginally incremental, or lacking in significance.** Manuscripts describing properties of crude extracts, without detailing the chemical composition of the extracts responsible for the described properties, will generally not be accepted for review.

All manuscripts submitted are reviewed and handled by the Editor-in-Chief or assigned to one of the Associate Editors. The Associate Editor and local Editorial Assistant are then responsible for the assigned manuscripts, including acknowledging receipt, evaluating the content and format of the paper, selecting reviewers, monitoring the progress of the review process, evaluating the comments of reviewers and forwarding them to the authors for their response, communicating ultimate acceptance or rejection to the corresponding authors, and carrying out a final check of accepted manuscripts for appropriate format and style.

Typically, three reviewers are selected per paper on the basis of the subject matter, available expertise, and the Editor's knowledge of the field. Potential reviewers for each paper are identified by various means, including a computerized search of the subject area. Authors must submit the names and addresses (including e-mail addresses and fax numbers) of at least four potential reviewers; however, the Editors are under no obligation to use specific individuals. Reviewers are normally asked to provide their assessments within two to three weeks. Anonymous copies of the reviews and the Editor's decision regarding the acceptability of the manuscript are sent to the corresponding author. If the reviewers' evaluations of the manuscript disagree, or if reviewer's and Editor's comments are not satisfactorily addressed by the authors, the Editor may reject the manuscript or select additional reviewers. These additional reviews are used by the Editor to assist in reaching the final decision regarding disposition of the manuscript.

The obligations of the Editors and Reviewers are outlined in the *Ethical Guidelines*.

Documents accepted for publication will be **posted on the *Journal's* ASAP website** as soon as they are ready for publication, that is, when the author's galley proof corrections have been made and all author concerns are resolved. This can occur anywhere from 2 to 8 weeks in advance of the cover date of the printed issue. Authors should take this into account when planning their intellectual and patent activities related to a document. The actual date on which the document is posted on the web is recorded in a separate line at the bottom of the first page of the document in the issue.

MANUSCRIPT PREPARATION

Manuscript Format. Manuscripts must be prepared using accepted word-processing software, and all parts must be double-spaced. All pages must be numbered consecutively starting with the title page and including tables and figures. PDF submissions must include line numbers at the left for the abstract and text, but no line numbers on tables. **Do not include line numbering on Word files;** Paragon Plus inserts line numbers during conversion to pdf. A standard font, in a size of 12 points or greater, must be used. The *Journal* requires authors to stay within a **20 typed page limit**, not including references, tables, and figures.

Standard American English usage is required. Authors who are not familiar with standard American English are urged to seek assistance; deficiencies in grammar may be a serious hindrance during the review process.

The ACS Style Guide (3rd ed., 2006; ISBN 0-8412-3999-1), available from Oxford University Press, Order Department, 201 Evans Road, Cary, NC 27513, provides a detailed treatment of the fundamentals of manuscript preparation. Refer to a current issue of the *Journal* for general style.

The various sections of the manuscript should be assembled in the following sequence:

- Title and authorship (single page)
- Abstract and keywords (single page)
- Introduction
- Materials and Methods
- Results
- Discussion
- Abbreviations Used
- Safety
- Acknowledgment
- Supporting Information description
- Literature Cited
- Figure captions
- Tables
- Figures
- Graphic for table of contents (optional)

TITLE AND AUTHORSHIP

The title, authorship, and institutional affiliations should be included on a single page.

Title. The title should be specific and informative. Keywords in the title assist in effective literature retrieval. If a plant is referred to in the title or elsewhere in the text by its common or trivial name, it should be identified by its scientific name in parentheses immediately following its first occurrence. This term should also be provided as one of the keywords. If trade names are mentioned, give generic names in parentheses.

Authorship. Be consistent in authorship designation on the manuscript and on all correspondence. **First name, middle initial, and last name** are generally adequate for correct identification, but omit titles. Give the complete mailing address of all institutions where work was conducted and identify the affiliation of each author. If the current address of an author is different, include it in a footnote on the title page. The name of the author to whom inquiries about the paper should be addressed must be marked with an asterisk; provide the telephone and fax numbers and e-mail address of this correspondent.

ABSTRACT AND KEYWORDS

Abstract. Authors' abstracts are used directly for *Chemical Abstracts*. The abstract should be a clear, concise (100–150 words), one-paragraph summary, informative rather than descriptive, giving scope and purpose, experimental approach, significant results, and major conclusions. Write for literature searchers as well as journal readers.

Keywords. Provide significant keywords to aid the reader in literature retrieval. The keywords are published immediately before the text, following the abstract.

INTRODUCTION

Discuss relationships of the study to previously published work, but do not reiterate or attempt to provide a complete literature survey. **The purpose or reason for the research being reported, and its significance, originality, or contribution to new knowledge in the field, should be clearly and concisely stated.**

Do not include or summarize current findings in this section.

MATERIALS AND METHODS

Apparatus, reagents, and biological materials used in the study should be incorporated into a general section. List devices of a specialized nature or instruments that may vary in performance, such that the model used may affect the quality of the data obtained (e.g., spectroscopic resolution).

List and describe preparation of special reagents only. Reagents normally found in the laboratory and preparations described in standard handbooks or texts should not be listed.

Specify the source, vendor [city and state (or city and country if non-U.S.)], and availability of special equipment, reagents, kits, etc. Do not include catalog numbers.

Biological materials should be identified by scientific name (genus, species, authority, and family) and cultivar, if appropriate, together with the site from which the samples were obtained. Specimens obtained from a natural habitat should be preserved by deposit of samples in an herbarium for plants or in a culture collection for microorganisms, with a corresponding collection or strain number listed.

Manuscripts describing studies in which live animals or human subjects are used must include 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** (see Reporting Specific Data: Animal or Human Studies).

Specific experimental methods should be sufficiently detailed for others to repeat the experiments unequivocally. Omit details of procedures that are common knowledge to those in the field. Brief highlights of published procedures may be included, but details must be left to the Literature Cited. Describe pertinent and critical factors involved in reactions so the method can be reproduced, but avoid excessive description. For information on the reporting of certain types of data see Reporting Specific Data.

Describe statistical design and methods in this section.

RESULTS/DISCUSSION

Results and discussion may be presented in separate sections or combined into a single section, whichever format conveys the results in the most lucid fashion. Be complete but concise in discussing findings, comparing results with previous work and proposing explanations for the results observed.

All data must be accompanied by appropriate statistical analyses, including complete information on sampling, replication, and how the statistical method employed was chosen.

Avoid comparisons or contrasts that are not pertinent, and avoid speculation unsupported by the data obtained.

A separate summary or conclusion section is not to be used; any concluding statements are to be incorporated under Results and Discussion.

ABBREVIATIONS AND NOMENCLATURE

Standard abbreviations, without periods, should be used throughout the manuscript.

Refer to *The ACS Style Guide* for the preferred forms of commonly used abbreviations. Specialized abbreviations may be used provided they are placed in parentheses after the word(s) for which they are to substitute at first point of use and are again defined in this section. Avoid trivial names and "code" abbreviations (e.g., NAR for naringenin) unless such codes are in common usage (e.g., MTBE for methyl *tert*-butyl ether).

If trade names are used, define at point of first use. If nomenclature is specialized, include a "Nomenclature" section at the end of the paper, giving definitions and dimensions for all terms. Use SI units insofar as possible. Refer to *The ACS Style Guide* for lists of SI units and a discussion of their use.

Write all equations and formulas clearly and number equations consecutively. Place superscripts and subscripts accurately; avoid superscripts that may be confused with exponents. Identify typed letters and numbers that might be misinterpreted, such as "oh" for zero or "ell" for one. Chemistry numbering requiring primes should be identified as such, not by a comma; e.g. 3,3'-hydroxy-.

It is the authors' responsibility to provide correct nomenclature. All nomenclature must be consistent and unambiguous and should conform with current American usage. Insofar as possible, authors should use systematic names similar to those used by Chemical Abstracts Service, the International Union of Pure and Applied Chemistry, and the International Union of Biochemistry and Molecular Biology. Chemical Abstracts (CA) nomenclature rules are described in Appendix IV of the *Chemical Abstracts Index Guide*. For CA nomenclature advice, consult the Manager of Nomenclature Services, Chemical Abstracts Service, P.O. Box 3012, Columbus, OH 43210-0012. A name generation service is available for a fee through CAS Client Services, 2540 Olentangy River Road, P.O. Box 3343, Columbus, OH 43210-0334 [telephone (614) 447-3870; fax (614) 447-3747; e-mail answers@cas.org]. In addition, the ACS website has links to nomenclature recommendations at <http://chemistry.org>.

SAFETY

Authors are required to call special attention in their manuscripts to safety considerations such as explosive tendencies, special precautionary handling procedures, and toxicity.

ACKNOWLEDGMENT

Include essential credits but hold to an absolute minimum. Omit academic and social titles. Meeting presentation data and acknowledgment of financial support of the work should not be included here; give these instead in a note following the Literature Cited.

LITERATURE CITED

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 30 or fewer citations.

Authors are responsible for the accuracy of their references. References taken from a review or other secondary source should be checked for accuracy with the primary source.

References should be listed on a separate sheet and numbered in the order in which they are cited in the text. References should be cited in the text by an on-line italic number in parentheses, 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".

Follow *Chemical Abstracts Service Source Index* for abbreviations of journal titles. Because subscribers to the Web edition of the *Journal* are now able to click on the "Chemport"

or other tag following each reference to retrieve the corresponding abstract from various Web resources, reference accuracy is critical.

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. (Use issue number only if each issue of the periodical begins with page 1.)

For books:

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.

Papers should not depend for their usefulness on unpublished material, and excessive reference to material "in press" is discouraged. Reference to the authors' own unpublished work is permitted if the subject is of secondary importance to the manuscript in question, but any unpublished results of central importance must be described in sufficient detail within the manuscript. **If pertinent references are "in press" or unpublished for any reason, furnish copies to enable reviewers to evaluate the manuscript. An electronic copy of these materials should be uploaded according to the directions for review-only Supporting Information.**

TABLES AND ARTWORK

The tables and graphics (illustrations) should be inserted after the Literature Cited section.

Tables and figures should be carefully designed to maximize presentation and comprehension of the experimental data with superfluous information excluded. Useful information not directly relevant to the discussion may be included under Supporting Information.

Tables. Tables may be created using a word processor's text mode or table format feature. The table format feature is preferred. Ensure each data entry is in its own table cell. If the text mode is used, separate columns with a single tab and use a line feed (return) at the end of each row.

Tables should be numbered consecutively with Arabic numerals and should be grouped after the Literature Cited section. Footnotes in tables should be given letter designations and be cited in the table by italic superscript letters. The sequence of letters should proceed by row rather than by column. Each table should be provided with a descriptive heading, which, together with the individual column headings, should make the table, as nearly as possible, self-explanatory. In setting up tabulations, authors are requested to keep in mind the type area of the journal page (17.8 × 25.4 cm), and the column width (8.5 cm), and to make tables conform to the limitations of these dimensions. **Arrangements that leave many columns partially filled or that contain much blank space should be avoided.** Conversely, arrangements that include >20 columns should be broken into two tables if possible. If *significance of values* is to be indicated, use a lower case letter, on line, one space after the value.

Figures and Artwork. Insert the illustrations into the word-processing file following the Literature Cited. Artwork should be sequentially numbered using Arabic numbers. Schemes and charts may have titles and footnotes; figures should have captions.

For bar charts, bars with hatching patterns generally reproduce well. Bars that range in shading from light to dark gray to black can usually be reproduced successfully, although we do not recommend any more than two shades of gray. A legend needs to be included within the figure itself rather than the patterns or shades included in the caption.

For manuscripts containing gel patterns, use of a high-resolution digital scanner is recommended. Only high-quality digital reproductions will allow reviewers to correctly verify the experimental results. For an example of gel patterns see *J. Agric. Food Chem.* **2004**, *52*, 5717–5723, Figures 2 and 3.

Only readable and accurately represented images are acceptable; the **Editors reserve the option to reject images that do not satisfactorily support points made in the manuscript or that are not of satisfactory quality for publication.**

The quality of the illustrations printed in the *Journal* largely depends on the quality of the originals provided. Figures cannot be modified or enhanced by the journal production staff. Contrast is important. Remove all color from graphics, except for those graphics that are to be considered for publication in color (see paragraph below on color reproduction for details). Each figure or photograph should be properly labeled.

Illustrations must fit a one- or two-column format on the journal page. **For efficient use of journal space, single-column illustrations are preferred.**

	single (preferred)	double
minimum width		10.5 cm (4.13 in.)
maximum width	8.25 cm (3.25 in.)	17.78 cm (7 in.)
maximum depth	24 cm (9.5 in.)	24 cm (9.5 in.)

For best results, submit illustrations in the actual size at which they should appear in the journal. Illustrations that do not need to be reduced to fit a single or double column will yield the best quality. Lettering should be no smaller than 4.5 points. (Helvetica or Arial type works well for lettering.) Lines should be no thinner than 0.5 point. Lettering and lines should be of uniform density. Avoid the use of very large and very small lettering within the same figure.

If artwork that must be reduced will be submitted, use larger lettering and thicker lines so that, when reduced, the artwork meets the above-mentioned parameters.

Avoid using complex textures and shading to achieve a three-dimensional effect. To show a pattern, choose a simple crosshatch design.

Color photographs and artwork may be printed in the journal if the Editor approves of their use. Color illustrations should be submitted **only** if they are essential for clarity of communication. Reproduction of color illustrations will be provided at no cost to the author; however, a surcharge of \$100 per 100 reprints will be added to the standard cost of reprints. Do not submit color prints to be printed in black and white.

Structural Formulas. Authors should note that structural formulas are valuable in expressing concisely the precise nature of the compounds under discussion and revealing the essence of the subject to readers unfamiliar with the topic, without their necessary recourse to reference materials. The use of chemical names without accompanying structures may cause readers to overlook the significance of the paper.

Structures should be produced with the use of a drawing program such as ChemDraw. Structure drawing preferences (preset in the ACS Stylesheet in ChemDraw) are as follows:

as drawing settings select	
chain angle	120°
bond spacing	18% of width
fixed length	14.4 points (0.508 cm, 0.2 in.)
bold width	2.0 points (0.071 cm, 0.0278 in.)
line width	0.6 point (0.021 cm, 0.0084 in.)
margin width	1.6 points (0.056 cm, 0.0222 in.)
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%

Using the ChemDraw ruler or appropriate margin settings, create structure blocks, schemes, and equations having maximum widths of 11.3 cm (one-column format) or 23.6 cm (two-column format). Note: if the foregoing preferences are selected as cm values, the ChemDraw ruler is calibrated in cm. Also note that a standard sheet of paper is only 21.6 cm wide, so all graphics submitted in two-column format must be prepared and printed in landscape mode.

Use boldface type for compound numbers but not for atom labels or captions.

Authors using other drawing packages should, as far as possible, modify their program's parameters to reflect the above guidelines.

TABLE OF CONTENTS GRAPHICS

Authors may include a suitable graphic for publication in the table of contents (TOC) in the Web edition of the *Journal*. **Submission of this graphic is optional.** This graphic should capture the reader's attention and, in conjunction with the manuscript's title, should give the reader a quick visual impression of the type of chemistry described. Structures in the TOC graphic should be constructed as specified under Structural Formulas above. The TOC graphic may be up to 4.7 in. (12.0 cm) wide and 1.8 in. (4.6 cm) tall. (See detailed instructions at the Paragon Plus website.) Text should be limited to labels for compounds, reaction arrows, and figures. The use of color to enhance the scientific value is acceptable. The TOC graphic should be inserted on a separate page at the end of the manuscript file.

SUPPORTING INFORMATION

Extensive tables, graphs, spectra, calculations, and other material beyond a modest content in the printed paper may be included in the Web edition of the journal. These will **not** be part of the printed article but can be accessed separately on the web by readers.

Supporting Information is uploaded as a separate file, as specified by the manuscript submission system, at the time the manuscript is submitted.

The material should be described in a paragraph inserted between the Acknowledgment and the Literature Cited sections, using the following format: "Supporting Information Available: Description. This material is available free of charge via the Internet at <http://pubs.acs.org>."

Components of the Supporting Information should be clearly labeled.

DO NOT UPLOAD FIGURES AND TABLES THAT ARE TO BE PUBLISHED IN THE ARTICLE INTO THE SUPPORTING INFORMATION FILE. Figures and tables that will appear in the published article are to be inserted in the manuscript directly after the Literature Cited section.

CURRENTLY ACCEPTABLE WORD-PROCESSING PACKAGES

Refer to the Paragon Plus Environment website (<http://pubs.acs.org/paragonplus/submission/software.html>).

LaTeX users should follow the guidelines given at <http://pubs.acs.org/paragonplus/submission/tex.html>.

WORD-PROCESSING DETAILS

When preparing a manuscript, use the document mode or its equivalent in the word-processing program, that is, do not save files in "Text Only" (ASCII) mode. If a non-Western version of the word-processing software is used to prepare the manuscript, save the file in rich-text format (RTF). Do not include any page-layout instructions such as placement information for graphics in the file. The text should be left justified, and automatic end-of-line hyphenation should be turned off. Use carriage returns only to end headings and paragraphs, not to break lines of text. Do not insert spaces before punctuation. To ensure expeditious processing of a manuscript, the references should conform to the format described under Literature Cited. Ensure that all characters are correctly represented throughout the manuscript: for example, 1 (one) and l (ell), 0 (zero) and O or o (oh), x (ex) and × (times sign). Check the final copy carefully for consistent notation and correct spelling. The editorial office conversion program will faithfully translate any errors to the typeset copy.

All of the text (including the title page, abstract, all sections of the body of the paper, figure captions, scheme or chart titles and footnotes, and references) and tabular material should be in one file, with the complete text first followed by the tabular material. It is best to use the fonts "Times" and "Symbol". Other fonts, particularly those that do not come bundled with the system software, may not translate properly. Ensure that all special characters (Greek characters, math symbols, etc.) are present in the body of the text as characters and not as graphic representations. Consult the documentation for the specific software package being used on how to detect the presence of graphics in the files and replace them with the appropriate text characters.

As additional features become available, these instructions will be updated at the *Journal's* website.

REVISIONS AND RESUBMISSIONS

For all revisions:

- Clearly identify the manuscript as a revision; reference the manuscript number.
- Include an itemized list of changes, with a response to each comment made by the Editor and by each reviewer.
- Be aware that the manuscript may be sent for additional review, at the discretion of the Editor.
- **Please fax the copyright status form to the assigned Editor.**

For all resubmissions:

- Clearly identify all resubmissions; reference the previous manuscript number.
- Include an itemized list of changes, including a response to each comment made by the Editor and by each reviewer.
- Indicate the three most appropriate journal sections for the article; a list of sections appears in the Journal Scope section of these instructions, and also at the Paragon Plus manuscript submission website. Final decision on the category under which the manuscript will be listed lies with the Editor.
- **Please fax the copyright status form to the assigned Editor.**

COPYRIGHT STATUS FORM

The ACS Copyright Status Form must be completed and signed for each submitted manuscript. No substitute forms or attachments are acceptable. A copy of this form can be found

on the ACS Paragon Plus website. The ACS Copyright Status Form is a legal document and must be signed manually. Once the form has been signed, it may be faxed or mailed to the Editor's office. Authors also have the option of uploading a PDF or TIF version of the signed form at the time of submission. The Completed and Signed Copyright Form file designation should be selected. **For questions about the form or about signing the form, contact the ACS Copyright Office at (202) 872-4368 or -4367.**

Note: Authors who are not U.S. government employees or bona fide agents should sign the top portion of the form only. If ALL of the authors were employees or bona fide agents of the U.S. government when the paper was prepared, the work is "a Work of the U.S. Government" and only the lower section, "Certification as a Work of the U.S. Government", should be signed if BOTH of the following circumstances apply:

- ALL authors are or were bona fide officers or employees of the U.S. Government when the paper was prepared.
- The work is a "Work of the U.S. Government", prepared by an officer/employee of the U.S. government as part of official duties.

If the work was prepared under a U.S. government contract or is coauthored by a non-U.S. government employee, the work is not a "Work of the U.S. Government"; DO NOT SIGN THIS LOWER SECTION. Sign only the top part of the form, on the line marked with the pointing hand. Call the ACS Copyright Office at the above telephone number for assistance.

PROOFS AND REPRINTS

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REPORTING SPECIFIC DATA

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)].

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, 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.

Proton Magnetic Resonance (PMR or ¹H NMR) Spectra. The frequency used, the solvent, and also temperature (if other than ambient) 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.

As an example that would be PMR for ethanol (60 MHz, CCl₄): δ 1.22 (t, 3, *J* = 7 Hz, CH₂CH₃), 2.58 (s, 1, OH), 3.70 (qd, 2, *J* = 7 Hz, OCH₂CH₃).

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, ¹H and ¹³C 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 $\mu\text{g}/\text{kg}$, 1–10 $\mu\text{g}/\text{kg}$, and 10–100 $\mu\text{g}/\text{kg}$ 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://soils.usda.gov/technical/classification/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.

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.

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, including a checklist of Institutional Animal Use and Care Committees (IUCAC) guidelines, is available at http://www.aphis.usda.gov/animal_welfare/publications_and_reports.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/frame_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/humansubjects/guidance/45cfr46.htm#46,htm#46.116>. 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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