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Authors whose manuscripts are published in *Journal of Agricultural and Food Chemistry* will be expected to review manuscripts submitted by other researchers from time to time.

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The *Journal of Agricultural and Food Chemistry* publishes high-quality, cutting edge original research representing complete studies and research advances 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. As a general rule, manuscripts dealing with herbal remedies or those testing specific compounds in cell-based assays related to disease states (e.g., “anticancer” activity) will no longer be considered within the scope of the *Journal* and should be submitted elsewhere. Manuscripts describing properties of extracts, without detailing the chemical composition of the extracts responsible for the described properties, will generally not be accepted for review.

The *Journal* is organized into the following sections:

Agricultural and Environmental Chemistry: crop protection chemistry, addressing synthesis combined with testing of new materials, environmental behavior and fate, residues, and mechanism of effects on both target and nontarget organisms.

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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.

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. Fragmentation of work into an incremental series of manuscripts is not acceptable.

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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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All manuscripts submitted are reviewed and handled by the Editor-in-Chief or assigned to one of the Associate Editors. The Associate Editor and Editorial Assistant are then responsible for the assigned manuscripts, including evaluating the content and format of the paper, selecting reviewers, monitoring the progress of the review process, evaluating the comments of reviewers

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Discuss relationships of the study to previously published work, but do not reiterate or attempt to provide a complete literature survey. Use of *Chemical Abstracts/Scifinder* and other appropriate databases is encouraged to ensure that important prior publications or patents are cited and that the manuscript does not duplicate previously published work. **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.**

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Describe statistical design and methods in this section.

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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 without redundancy. Be complete but concise in discussing findings, comparing results with previous work and proposing explanations for the results observed.

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

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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).

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It is the authors' responsibility to provide correct nomenclature. Structures should be included for uncommon chemicals, particularly when the systematic or common name is too complex or unclear to readily denote the structure. Such structures should be included as a figure or table. 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

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ACKNOWLEDGMENT

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REFERENCES

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 listed on a separate page and numbered in the order in which they are cited in the text.

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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. (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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The tables and graphics (illustrations) should be inserted in the manuscript file after the References section. Do not upload tables and graphics that are to be published with the manuscript as Supporting Information files.

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. Lower case should be used for all table entries unless a capital letter is required. If the text mode is used, separate columns with a single tab and use a line feed (enter) at the end of each row.

Tables should be numbered consecutively with Arabic numerals and should be grouped after the figure captions. 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.

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For manuscripts containing gel patterns, use of a high-resolution digital scanner is recommended. Only high-quality original, unaltered 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.

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The quality of the illustrations published 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. Each figure or photograph should be properly labeled.

Graphics should be sized at the final production size when possible. Single-column graphics are preferred and can be sized up to 240 points (3.33 in.). Double-column graphics must be sized between 300 and 504 points (4.167 in. and 7 in.). All graphics have a maximum depth of 660 points (9.167 in.) including the caption (please allow 12 points for each line of caption text). Consistently sizing letters and labels in graphics throughout the manuscript will help to ensure consistent graphic presentation for publication. 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.

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

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. Do not submit color prints to be printed in black and white.

Structural Formulas. Structural formulas should be included for all new chemicals and for existing chemicals for which chemical nomenclature and/or trivial names do not convey the structure adequately. 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.

For more information, please visit <http://pubs.acs.org/page/4authors/submission/index.html>.

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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 (^1H 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 ^1H NMR for ethanol (60 MHz, CCl_4): δ 1.22 (t, 3, $J = 7$ Hz, CH_2CH_3), 2.58 (s, 1, OH), 3.70 (qd, 2, $J = 7$ Hz, OCH_2CH_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](https://doi.org/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 ^{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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