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JOURNAL OF AGRICULTURAL AND FOOD CHEMISTRY

Scope • Policy • Instructions for Authors

(Revised January 2016)

Contents *(click on the topic)*

1. IMPORTANT MANUSCRIPT SUBMISSION REQUIREMENTS

Manuscripts and revised manuscripts must be submitted via the ACS Paragon Plus Web site (http://paragonplus.acs.org/login). E-mailed submissions and hardcopy submissions will not be processed. An overview of and complete instructions for the Web submission process are available at the ACS Paragon Plus Web site.

When submitting, please be aware of the following requirements:

- All manuscripts must be accompanied by a **cover letter** that includes an **explicit statement on the manuscript's significance** (not a summary of the abstract), including its originality, its contribution to new knowledge in the field, and its relevance to research in agricultural and food chemistry.

- All **coauthors** listed on the title page of the manuscript must be entered into the Paragon Plus System at step 2 in the manuscript submission process. Only one corresponding author is allowed for each manuscript in Paragon Plus. Additional corresponding authors may be designated on the manuscript title page. Use of the phrase "all authors contributed equally" is discouraged. Instead, statements about author contributions should identify the specific aspect of the author's contribution.

- The **manuscript abstract and text** must appear in a single, double-spaced column; lines in the abstract and text must be numbered consecutively from beginning to end in a separate column at the left. There is **no separate conclusion section** to be used; conclusions should be incorporated into the results and discussion section. All of the manuscript text (including 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.

- To ensure that a submitted manuscript meets **sufficient interest of the readership** of the journal, it is expected that articles recently published on the respective topic in the *Journal of Agricultural and Food Chemistry* are cited to a reasonable extent. In general, **references** must be numbered in the order in which they appear in the text.

- The author's preference for **manuscript category** is indicated during the submission process. However, the final decision on the category under which the manuscript will be listed lies with the Editor.

- The system requires authors to supply the names, e-mail addresses, and affiliations of at least **four recommended reviewers**. The recommended reviewers should be experts in the subject matter of the manuscript and not be anyone who is or has been a former adviser/advisee, colleague in the same institution, research collaborator, and/or coauthor of papers and patents or in any other way has a conflict of interest.

- If the manuscript is one of a series of **companion manuscripts** that will be published sequentially, please describe the planned series in the cover letter, mentioning previously published parts and giving an estimate of when subsequent parts will be submitted.

- Authors selecting the ***Just Accepted*** manuscript option when submitting should be sure that the form of author and coauthor names as entered into the Paragon Plus System is identical to the form on the manuscript title page.

Complete instructions for manuscript preparation and the Journal Publishing Agreement form are updated frequently and are available at the *Journal's* Web site. Please conform to these instructions when submitting manuscripts.

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.

2. JOURNAL SCOPE

The *Journal of Agricultural and Food Chemistry* considers high-quality, original research representing complete studies and scientific advances dealing with the innovative application of chemistry, biochemistry and biological sciences to increase the molecular understanding of product attributes, processes, technologies, and health aspects encompassing the agricultural-food-nutrition continuum.

Manuscripts are expected to involve chemistry, biochemistry and/or molecular biology as the fundamental component and can be combined with novel aspects of process engineering and food technology, authenticity and origin aspects of food, or the biological evaluation of agricultural systems including plant-plant, plant-fungal and plant-insect interactions, and/or food systems. The latter may include microbial, nutritional, physiological, sensory, or toxicological properties, and data must accompany sufficient discussion to demonstrate their relevance to food and nutrition.

Research considered for publication should be of general interest to the scientific community and/or the public, its potential impact should be significant and the technical quality is expected to conform to the highest standards of chemical research.

Current specific categories are as follows:

- Agricultural and Environmental Chemistry
- Bioactive Constituents, Metabolites, and Functions
- Biofuels and Bio-based Materials
- Biotechnology and Biological Transformations
- Chemistry and Biology of Aroma and Taste
- Food and Beverage Chemistry/Biochemistry
- Food Safety and Toxicology
- Functional Structure/Activity Relationships
- New Analytical Methods
- Omics Technologies Applied to Agriculture and Food

These categories are periodically reviewed and may be changed.

3. JOURNAL CATEGORIES

• Agricultural and Environmental Chemistry

to advance molecular knowledge (e.g., crop protection chemistry, nanotechnology, natural toxins, fate and biotransformation of residues), elucidate mechanisms of action of agrochemicals, understand mechanisms of plant-plant, plant-fungal and plant-insect interactions including the action of bioactive constituents in desirable plants on control of pests that threaten them, and promote innovative solutions for increased agricultural productivity, a sustainable supply of food and fiber, and protection of public health and the environment including water quality/treatment, agricultural waste, and energy-related issues.

• Bioactive Constituents, Metabolites, and Functions

to increase knowledge of chemical structures of bioactive constituents, phytonutrients, and nutraceuticals in foods, their human and animal metabolism, and their mechanisms of biological function to affect human health status, including various aspects of molecular nutrition such as nutritional biochemistry, nutrigenomics and metabolomics. Studies on traditional medicines and herbal remedies are outside the scope of this category. It is mandatory that manuscripts reporting on biological properties of crude extracts include detailed information on the chemical composition of the extracts causing the described properties.

Manuscripts can encompass cell-based or other in vitro assays, animal models, clinical human trails, or a combination thereof as the fundamental component, however, test systems applied must be appropriate and the analytical method used should allow the quantitation of time and dose response effects. It is understood that discussion on nutritional relevance and conclusions on human health aspects are carefully formulated considering the experimental design used (appropriate cell test lines, significance of test/trail, relevant dose levels) and the data obtained.

• Biofuels and Biobased Materials

to advance knowledge of chemistry, biology, and processing of biobased products and biofuels including all the related areas of biodiesel, bioethanol, biogas, biotransformations and bioprocesses (plants, algae etc.), waste utilization, biorefinery and bioresource technologies associated with conversion or production of biobased materials, and sustainability, and environmental emissions and effects associated with these processes.

• Biotechnology and Biological Transformations

to foster technological advances in plant/agricultural biotechnology (e.g., crop improvement, nutraceuticals, bioenergy, transgenic plants, phytoremediation), microbial and insect biotechnology (metabolic engineering and synthetic/systems biology of bacteria, fungi, insects, yeasts and algae in the context of fermentation/bioproduction, biocatalysis, bioremediation, biodegradation), food and flavor biotechnology (biotransformations/microbiology and metabolic aspects of food/beverage systems), and protein and enzyme technology (recombinant proteins/enzymes, cell-free protein expression systems, and biocatalysis using immobilized enzymes).

• Chemistry and Biology of Odor and Taste

to advance molecular knowledge of the instrumental analysis (e.g. bioelectronics sensors), chemical structures, and formation pathways of aroma and taste molecules of plant and animal derived foods and beverages, the chemosensory receptors mediating flavor object recognition (e.g. *in vitro* cell assays), human *in vivo* psychophysics (incl. multisensory integration), and neurological processing of flavor stimuli (imaging technologies).

• Food and Beverage Chemistry/Biochemistry

to deepen the fundamental understanding of chemical structures, structural modifications, interactions, and (bio)chemical transformations of minor and major components in foods and beverages, potentially in combination with novel aspects of process engineering, food technology, nanotechnology, packaging and storing, authenticity and origin aspects of food, or the biological evaluation of food and beverage systems.

• Food Safety and Toxicology

to advance our knowledge of detrimental health effects and the mechanisms of adverse physiological, or pathological changes induced by natural or synthetic chemicals occurring in the human environment with particular emphasis on foods, crop protection chemicals, contaminants and related chemicals (e.g., nanomaterials, biotechologically derived products), including agricultural safety and consumer product safety, and the design and action of chemically related processes that enhance food safety.

• Functional Structure/Activity Relationships

to increase the knowledge on the relationship between chemical structure and biological (microorganisms, insects, animals, human) or technofunctional activity (e.g., Emulsifying, foaming, gelation) of agricultural and food components.

This category comprises (i) organic synthetic studies and/or structural biological studies (X-ray, NMR, etc.) of relevant ligands and targets with the aim of investigating molecular recognition processes in the action of biologically active compounds, (ii) molecular biological studies (e.g., site-directed mutagenesis) of macromolecular targets that lead to an improved understanding of molecular recognition, and (iii) computational studies that analyze the SAR of compounds of interest and lead to experimental studies or analysis of other available chemical and/or biological data that substantially advance the knowledge in agricultural and food chemistry.

Routine extensions of existing series that do not add significantly to a basic understanding of the structure-activity relationship (SAR) of the series or do not utilize novel chemical/biological approaches will normally not be considered for publication.

- **New Analytical Methods**

to expand the repertoire of analytical methods in agriculture and food research by new analytical method development using chemical, physical, and biological principles. Manuscripts dealing with existing analytical methods should offer a significant, original application of the method or a major improvement going far beyond state-of-the-art.

For manuscripts describing the application of an existing method, even when modified, the category selected should be driven by the application (e.g., Agricultural and Environmental Chemistry, Bioactive Constituents, Metabolites, and Functions, etc.).

- **Omics Technologies Applied to Agriculture and Food**

to promote a more integrative understanding of complex systems in agriculture, food, and nutrition by the application of metabolomics, proteomics, and transcriptomics/genomics technologies combined with, but not limited to, bioinformatics and computational biology.

It is mandatory that manuscripts in this category go beyond a sheer holistic fingerprinting of samples, i.e. metabolic changes need to be identified on a molecular level and validated by means of targeted analysis.

4. 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 and/or molecular biology**. Novel experimental results, theoretical treatments, interpretations of data, and absence of prior publications on the same/similar topics will document originality. Fragmentation of work into an incremental series of manuscripts is not acceptable.

• **LETTERS** are manuscripts describing results deemed to be highly important and urgent in a field of research. **Only manuscripts reporting complete research, as opposed to preliminary results, will be considered.** The cover letter for these manuscripts must clearly describe why the results are timely and urgent enough to justify the Letters format. In addition, the abstract must also make this plain to the reader. If deemed appropriate by the editors for the format, these manuscripts will be subject to the normal, but expedited, peer review process.

• **REVIEW ARTICLES** will be considered that comprehensively summarize information in a field in which the literature is scattered and/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 may contact the Editor with any questions.

• **PERSPECTIVES** are expected to explore needs and opportunities in agricultural and food chemistry in a less technical format than a Review Article. Authors are invited to contact the Editor with any questions before submitting a Perspectives manuscript. For an example, see *J. Agric. Food Chem.,* 2013, 61, 1155–1159 (DOI:10.1021/jf305122s). Perspectives summarizing highlights of symposia will also be considered. For an example, see *J. Agric. Food Chem.* **2013**, *61*, 4676-4691 (DOI: 10.1021/jf305281c).

• **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.,* **2015**, 63, 5305–5306 (DOI: 10.1021/jf506172q) and J. Agric. Food Chem., **2015**, 63, 5307–5307 (DOI: 10.1021/acs.jafc.5b01143).

• **ADDITIONS/CORRECTIONS** may be used to address important issues or correct errors and omissions of consequence that arise after publication of an article. Additions and Corrections may be requested by the author(s) or initiated by the Editor after discussions with the corresponding author. Readers who detect errors of consequence in the work of others should contact the corresponding author of that work. All Additions and Corrections are subject to approval by the Editor, and minor corrections and additions will not be published. Additions and Corrections from authors should be submitted via the ACS Paragon Plus environment by the corresponding author for publication in the "Addition/Correction" section of the Journal. The corresponding author should obtain approval from all of the article coauthors prior to submitting an Addition and Correction or provide evidence that such approval has been solicited. The Addition and Correction should include the original article title and author list, citation including DOI, and details of the correction. For proper formatting, see examples in a current issue of the Journal.

SYMPOSIA or TOPICAL COLLECTIONS comprise 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. Each manuscript will be subject to the normal peer-review process. For an example, see *J. Agric. Food Chem.,* **2015**, 63, 5837–5840 (DOI: 10.1021/acs.jafc.5b00324) and J. Agric. Food Chem., **2015**, 63, 5099–5099.(DOI: 10.1021/acs.jafc.5b00159)

RETRACTION of articles may occur for scientific or ethical reasons. Articles that contain seriously flawed or erroneous data such that their findings and conclusions cannot be relied upon may be retracted to correct the scientific record. Retractions may be requested by the article author(s) or by the journal Editor(s), but are ultimately published at the discretion of the Editor. When an article is retracted, a notice of retraction will be published containing information about the original article title, author list, and the reason for the retraction. Retracted articles will be accompanied by the related retraction notice and will be marked as "Retracted". The originally published article will remain on the web except in extraordinary circumstances (e.g., when deemed legally necessary or if the availability of the published content poses public health risks). The American Chemical Society follows guidance from the Committee on Publication Ethics (COPE) when considering retractions; for more information see http://publicationethics.org/.

5. ETHICS & CONFLICT OF INTEREST

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

Authors and coauthors should familiarize themselves by carefully reading the *Ethical Guidelines to Publication of Chemical Research*, which is available at the ACS Publications Web site.

A statement describing any financial conflicts of interest or lack thereof is published with each manuscript. During the submission process, the corresponding author must provide this statement on behalf of all authors of the manuscript. The statement should describe all potential sources of bias, including affiliations, funding sources, and financial or management relationships, that may constitute conflicts of interest (please see http://pubs.acs.org/ethics, ACS Ethical Guidelines). The statement will be published in the final paper. If no conflict of interest is declared, the following statement will be published in the paper: "The authors declare no competing financial interest."

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6. AUTHOR LIST & OPEN RESEARCHER AND CONTRIBUTOR ID (ORCID)

During manuscript submission, the submitting author must provide contact information (full name, e-mail address, institutional affiliation and mailing address) for all of the co-authors. Because all of the author names are automatically imported into the electronic Journal Publishing Agreement, the names must be entered into ACS Paragon Plus in the same sequence as they appear on the first page of the manuscript. (Note that co-authors are not required to register in ACS Paragon Plus.) The author who submits the manuscript for publication accepts the responsibility of **notifying all co-authors that the manuscript is being submitted**. Deletion of an author after the manuscript has been submitted requires a confirming letter to the Editor-in-Chief from the author whose name is being deleted. For more information on ethical responsibilities of authors, see the Ethical Guidelines to Publication of Chemical Research.

All authors are strongly encouraged to register for an ORCID iD, a unique researcher identifier. With this standard identifier, you can create a profile of your research activities to distinguish yourself from other researchers with similar names and make it easier for your colleagues to find your publications. Learn more at http://www.orcid.org. Authors and reviewers can add their ORCID iD to, or register for an ORCID iD from, their account in ACS Paragon Plus.

The ORCID Registry is available free of charge to individuals, who may obtain an ORCID identifier, manage their record of activities, and search for others in the ORCID Registry. Authors and reviewers can add their ORCID ID to, or register for an ORCID ID from, their account in ACS Paragon Plus. Submitting authors have the option to provide existing ORCID IDs for coauthors during submission, but they cannot create new ORCID IDs for coauthors.

7. EDITORIAL PEER REVIEW PROCESS

Peer review is used to help ensure the **highest possible quality** in published manuscripts. Scientists with expertise in the subject matter being treated will evaluate the manuscript for its originality and validity of the experimental design and results, the significance and impact in the field of agricultural and food chemistry, as well as the appropriateness to the *Journal*.

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 and forwarding them to the authors for their response, communicating ultimate acceptance or rejection to the corresponding author, and carrying out a final check of accepted manuscripts for appropriate format and style.

The Editors may exercise their prerogative to decline a manuscript after **editorial 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.

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) of at least four potential reviewers who do not have conflicts of interest with the authors or manuscript content; 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*. Aids for reviewers titled "A Guide to a Review" and "Components of a Manuscript to be Considered in a Review" are available at the Reviewer Information Web site (http://pubs.acs.org/4authors).

Manuscript Transfer Service

Occasionally editors in ACS Journals feel that manuscripts are a better fit for another ACS Journal and suggest that authors consider transferring the submission. The Manuscript Transfer Service simplifies and shortens manuscript submission to another ACS journal, as all the coauthors, suggested reviewers, manuscript files, and responses to submission questions are copied to the new submission. Once authors have selected a new journal, the journal office will facilitate the transfer to that journal.

To determine if a manuscript transfer is an appropriate next step, authors are encouraged to read "Is Manuscript Transfer Right for Me?" Authors are also reminded to review journal editorial scope statements as they consider the next destination for the submission.

Requirements of the next journal may be different, so authors should also check the Author Guidelines and make any needed revisions to conform to those requirements. Note that transferring a manuscript is not a guarantee that the manuscript will be accepted, as the final publication decision will belong to the Editor of the next journal. Please keep in mind that the reviews, reviewer identities, and decision letter will all be transferred to the next journal. For complete details, see http://pubs.acs.org/page/policy/manuscript_transfer/index.html.

***Just Accepted* Manuscripts.** *Just Accepted* manuscripts are peer-reviewed, accepted manuscripts that are published on the ACS Publications Web site prior to technical editing, formatting for publication, and author proofing—usually within 30 minutes to 24 hours of acceptance by the editorial office. During the manuscript submission process, authors can choose to have their manuscript published online as a *Just Accepted* manuscript. Authors choosing this option must ensure that all intellectual property/patent issues are resolved. To ensure rapid delivery of the accepted manuscript to the Web, authors must adhere carefully to all requirements in the journal's Scope, Policy, and Instructions for authors. For further information, please refer to the *Just Accepted* FAQ, at http://services.acs.org/pubshelp/passthru.cgi?action=kb&item=244. Note that publishing a manuscript as *Just Accepted* is not a means by which to comply with the NIH Public Access Mandate.

ASAP Publication. Accepted manuscripts will be published on the "Articles ASAP" page on the *Journal's* Web site as soon as page proofs are corrected and all author concerns are resolved. Publication on the Web usually occurs within 4 working days of receipt of page proof corrections, and this can be anywhere from 2 to 6 weeks in advance of the cover date of the issue. Manuscripts assigned to a special issue often remain published ASAP for several months. Authors should take this schedule into account when planning intellectual and patent activities related to a manuscript. The date on which an accepted paper is published on the Web is recorded on the Web version of the manuscript and on the first page of the PDF version.

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. **Lines in the abstract and text should be numbered consecutively from beginning to end in a separate column at the left. Do not put line numbers on pages with tables or figures.** A standard font, in a size of 12 points or greater, must be used. The *Journal* has a **20 typed page limit**, not including references, tables, and figures. Authors must request approval from the Editor in Chief to submit manuscripts exceeding 20 typed pages.

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.

Assistance with English Language Editing. Authors may want to have their manuscripts edited professionally before submission to improve clarity. The ACS ChemWorx English Editing Service can assist you in improving and polishing the language in your manuscript. You can learn more about the services offered, at http://es.acschemworx.acs.org.

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 style guide is also available at the Journal's Web site and through ACS ChemWorx.

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 (including Safety information)
Results/Discussion
Abbreviations Used
Acknowledgment
Supporting Information description
References
Figure captions
Tables
Figure graphics
Graphic for table of contents

TITLE, AUTHORSHIP, AND KEYWORDS

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

Title. The title should be specific, informative, and concise. 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 e-mail address of this correspondent.

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

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.

INTRODUCTION

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. Current findings should not be included or summarized in this section.**

MATERIALS AND METHODS

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

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 a 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. Authors are encouraged to note the approval code or number or give the**

name of the approving office or official. (See Reporting Specific Data: Animal or Human Studies.) Manuscripts reporting data from inhumane treatment of experimental animals will be rejected.

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 References, and verbatim repeat of previously published methods, even if done by the authors, will not be permitted unless a quotation from a published work is included, and placed in quotation marks, with the reference to the source included at the end of the quotation. 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 AND 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 without redundancy. 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 (i.e., 3,3´-dihydroxy-), not by an apostrophe (e.g., 3,3'-dihydroxy-).

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 to 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 Web site has links to nomenclature recommendations at http://chemistry.org.

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 References. It is the responsibility of the corresponding author to notify individuals named in the Acknowledgment prior to submission.

FUNDING SOURCES

When submitting a manuscript to the Journal via ACS Paragon Plus, the submitting author is asked to identify the funding sources for the work presented in the manuscript. Identifying funding sources is optional during submission of an original manuscript. Funding source information is required when a revised manuscript is submitted. Funding should be acknowledged in a separate statement (not in the Acknowledgment paragraph).

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. To demonstrate that the submitted manuscript meets sufficient interest of the readership of the journal, **it is expected that articles recently published on the respective topic in the *Journal of Agricultural and Food Chemistry* be cited to a reasonable extent**. As a general guideline, authors should attempt to limit the literature cited to approximately 50 or fewer citations (except for review or perspective manuscripts).

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 page and numbered in the order in which they are cited in the text.

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”.

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.)

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.

For Web pages:

3. Black, A.; White, B. Page title. URL (http://...) (most recent access date).

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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.

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Size	10 points
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A statement describing any financial conflicts of interest or lack thereof is published with each manuscript. During the submission process, the corresponding author must provide this statement on behalf of all authors of the manuscript. The statement should describe all potential sources of bias, including affiliations, funding sources, and financial or management relationships, that may constitute conflicts of interest (please see the *Ethical Guidelines*). The statement will be published in the final article. If no conflict of interest is declared, the following statement will be published in the article: "The authors declare no competing financial interest."

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12. REPORTING SPECIFIC DATA

Bioactivity. Manuscripts reporting on key bioactive constituents in agricultural products, foods, and beverages and on the mechanisms of how these compounds promote health in living organisms, including humans, livestock and domestic animals are expected to follow a cutting edge chemical, biochemical, and/or molecular biological approach.For the identification of a bioactive agricultural/food compound, an activity-guided fractionation approach should be followed, with generally accepted criteria for complete chemical characterization of the bioactive compound's molecular structure using state-of-the-art analytical tools (TOF-MS, 1D/2D-NMR etc.).

Manuscripts can encompass cell-based or other *in vitro* assays, animal models, human intervention studies, clinical trials, or a combination thereof as the fundamental component, however, target compounds need to be tested at relevant dose levels, test systems applied must be validated, should allow the quantitation of time and dose response effects, and need to be appropriate for *in vivo* conditions. In order to demonstrate bioefficacy as an overall aim of the 'Bioactives Research' theme, the bioavailability of the target food constituent has to be substantial and may, in some cases, not be sufficient to exert the desired effect after dietary intake. Therefore, the discussion on nutritional relevance and conclusions on human health aspects need to be carefully formulated considering the experimental design used (appropriate cell-based or other *in vitro* assays, animal models, clinical human trials, significance of test/trial, relevant dose levels etc.), the robustness of the data set obtained, and addressing the underlying mechanism of action.

It is mandatory that manuscripts reporting on biological properties of individual constituents include information on the purity of the test components and on how it has been determined (e.g., ^{1}H NMR, GC-FID, HPLC-ELSD). Similarly, investigations performed with crude extracts need to present detailed information on the chemical composition of the extracts responsible for the described properties. This means that key representatives of the chemical class investigated (e.g., polyphenols, terpenoids, alkaloids, peptides) should be quantitatively fingerprinted.

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 NMR, mass scpectrometric, or other spectral data 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 (DOI: 10.1021/jf034246+).
- 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 (DOI: 10.1021/jf049526j).
- 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 (DOI: 10.1021/jf040100e).

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) (DOI: 10.1021/jf960654k)]. 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) (DOI: 10.1021/jf034085+). A good example for aroma compound identification is (*J. Agric. Food Chem.*, **2000**, 48 (6), pp 2430–2437) (DOI: 10.1021/jf991116l).

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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