



Last updated: September 17, 2024 View the latest guidelines online

# **Manuscript Submission Requirements Checklist**

Manuscripts and revised manuscripts must be submitted via the ACS Paragon Plus Web site (<a href="acsparagonplus.acs.org">acsparagonplus.acs.org</a>). 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 website.

When submitting, please be aware of the following requirements:

- All manuscripts must be accompanied by a written statement on the manuscript's significance (not a summary of the abstract), addressing the following three bullet points:

  statement of the problem addressed and originality of the approach,
  contribution of the work to create new knowledge in the field, and
  relevance of the work to advance research and impact to the field of agricultural and food chemistry, including the specific role of molecular research in the study. This 3-point statement should be uploaded as an informal letter using the manuscript file designation "Supporting information for review only".
- All co-authors listed on the title page of the manuscript must be entered into the ACS
   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* and other similar journals in the field 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 co-author 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.

Complete instructions for manuscript preparation are updated frequently and are available at the *Journal*'s website. 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.

# Scope of the Journal

The <u>Journal of Agricultural and Food Chemistry</u> 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**

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, metabolic changes need to be identified on a molecular level and validated by means of targeted analysis.

These categories are periodically reviewed and may be changed.

# **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.

**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**, as opposed to a comprehensive Review Article, are expected to be concise discussions of a particular field to help readers keep abreast of the advances and trends in agricultural and food chemistry outside their own area of expertise. Therefore, Perspectives are written in a manner understandable to scientists working in any area under the broader umbrella of agricultural and food chemistry. Following an abstract of no more than 100 words, the text of the Perspective should not exceed 12 double-spaced manuscript pages in length, exclusive of tables, figures, photographs, and references. Up to four tables, figures, or photographs, total, may be

included.

**VIEWPOINTS** are short opinion-style manuscripts that provide authors with a venue to comment on an issue of pressing importance to the JAFC readership community. Viewpoints are not peer-reviewed but are subject to editorial approval. JAFC welcomes Viewpoints of a scientific nature; no Viewpoints of an exclusively political nature will be considered for publication. Successful Viewpoints clearly articulate a research need to the reader and avoid summarizing a particular research area or study. A limit of 1000 words + author affiliations + 1 single-frame figure with a 50 word caption OR a 350 word table will be strictly enforced; submissions exceeding this maximum will not be considered.

**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, not 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).

**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: <a href="https://doi.org/10.1021/acs.jafc.5b00324">10.1021/acs.jafc.5b00324</a>) and J. Agric. Food Chem., **2015**, 63, 5099–5099.( DOI: <a href="https://doi.org/10.1021/acs.jafc.5b00159">10.1021/acs.jafc.5b00159</a>).

# **ACS Researcher Resources**

While this document will provide basic information on how to prepare and submit the manuscript as well as other critical information about publishing, we also encourage authors to visit <u>ACS</u> <u>Researcher Resources</u> for additional information on everything that is needed to prepare (and review) manuscripts for ACS journals and partner journals, such as

- Mastering the Art of Scientific Publication, which shares editor tips about a variety of topics including making your paper scientifically effective, preparing excellent graphics, and writing cover letters.
- Resources on how to prepare and submit a manuscript to ACS Paragon Plus, ACS
   Publications' manuscript submission and peer review environment, including details on
   selecting the applicable <u>Journal Publishing Agreement</u>.
- Sharing your research with the public through the ACS Publications open access program.
- ACS Reviewer Lab, a free online course covering best practices for peer review and related ethical considerations.
- ACS Author Lab, a free online course that empowers authors to prepare and submit strong manuscripts, avoiding errors that could lead to delays in the publication process.
- ACS Inclusivity Style Guide, a guide that helps researchers communicate in ways that recognize and respect diversity in all its forms.

# **Manuscript Preparation**

#### **Submit with Fast Format**

All ACS journals and partner journals have simplified their formatting requirements in favor of a streamlined and standardized format for an initial manuscript submission. Read more about the requirements and the benefits these serves authors and reviewers <a href="here">here</a>.

Manuscripts submitted for initial consideration must adhere to these standards:

- Submissions must be complete with clearly identified standard sections used to report original research, free of annotations or highlights, and include all numbered and labeled components.
- Figures, charts, tables, schemes, and equations should be embedded in the text at the point of relevance. Separate graphics can be supplied later at revision, if necessary.
- When required by a journal's structure or length limitations, manuscript templates should be used.
- References can be provided in any style, but they must be complete, including titles. For information about the required components of different reference types, please refer to the ACS Style Quick Guide.
- Supporting Information must be submitted as a separate file(s).

## **Document Templates and Format**

The *Journal of Agricultural and Food Chemistry* does not require the use of any document templates. General information on the preparation of manuscripts may be found in the <u>ACS Guide to Scholarly Communication</u>.

# Acceptable Software, File Designations, and TeX/LaTeX

See the list of <u>Acceptable Software</u> and appropriate <u>File Designations</u> to be sure your file types are compatible with ACS Paragon Plus. Information for manuscripts generated from <u>TeX/LaTeX</u> is also available.

### **Cover Letter**

A cover letter must accompany every manuscript submission. During the submission process, you may type it or paste it into the submission system, or you may attach it as a file.

# **Manuscript Text Components**

### MANUSCRIPT FORMAT

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.

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
- Graphic for table of contents

## TITLE, AUTHORSHIP, AND KEYWORDS

**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 number and e-mail address of this correspondent.

Many Funders and Institutions require that institutional affiliations are identified for all authors listed in the work being submitted. ACS facilitates this requirement by collecting institution information during manuscript submission under Step 2: Authors and Affiliations in ACS Paragon Plus.

**Keywords.** Provide significant keywords to aid the reader in literature retrieval. Please consider the use of words different from those in the title to expand discoverability of the article. 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 must emphasize any unexpected, new, and/or significant hazards or risks associated with the reported work. This information should be in the experimental details section of the full article or communication.

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. 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.

### 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 <u>The ACS Style Guide</u> 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 <u>The ACS Style Guide</u> 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].

### **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**

Authors are required to report ALL funding sources and grant/award numbers relevant to the manuscript. Enter all sources of funding for ALL authors relevant to the manuscript BOTH in the Open Funder Registry tool in ACS Paragon Plus and in the manuscript to meet this requirement. See <a href="http://pubs.acs.org/page/4authors/funder\_options.html">http://pubs.acs.org/page/4authors/funder\_options.html</a> for complete instructions.

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* and other similar journals in the field are cited to a reasonable extent.

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:

• 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 )

#### For books:

• 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:

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

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. "In press" references should include the Digital Object Identifier (DOI) assigned by the potential publisher.

#### TABLES AND ARTWORK

Tables and figures should be carefully designed to maximize presentation and comprehension of the experimental data with superfluous information excluded. Tables must be self-contained, that is, understandable without reading the text of the article. This includes using footnotes to explain sample names, units, and other relevant information. 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.

**Figures and Artwork.** The preferred submission procedure is to embed graphic files in a Word document. It may help to print the manuscript on a laser printer to ensure all artwork is clear and legible. Artwork should be sequentially numbered using Arabic numbers. Schemes and charts may have titles and footnotes; figures should have captions. Insert the captions following the References and the graphics after the Tables.

Additional acceptable file formats are TIFF, PDF, EPS (vector artwork), or CDX (ChemDraw file). If submitting individual graphic files in addition to their being embedded in a Word document, ensure the files are named according to graphic function (i.e., Scheme 1, Figure 2, Chart 3), not the scientific name.

Labeling of all figure parts should be present, and the parts should be assembled into a single graphic. For EPX files, ensure that all fonts are converted to outlines or embedded in the graphic file. The document setting should be in RGB mode. **Note**: Although EPS files are accepted, the vector-based graphics will be rasterized for production. Please see below for TIFF file production resolutions.

TIFF files (either embedded in a Word document or submitted as individual files) should have the following resolution requirements: black and white line art, 1200 dpi; grayscale art (a monochromatic image containing shades of gray), 600 dpi; color art (RGB color mode), 300 dpi.

The RGB and resolution requirements are essential for producing high-quality graphics within the published paper. Graphics submitted in CMYK or at lower resolution may be used; however, the colors may not be consistent. Graphics of poor quality may not be able to be improved.

Most graphic programs provide an option for changing the resolution when images are saved. Best practice is to save the graphic file at the final resolution and size using the program used to create the graphic.

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 original, unaltered digital reproductions will allow reviewers to correctly verify the experimental results. For an example of gel patterns see *J. Agric. Food Chem.*, 2012, 60 (18), 4492–4499 (DOI: 10.1021/jf300563n).

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 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.

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 requirements (preset in the ACS Stylesheet in ChemDraw) are as follows:

- As drawing settings, select: chain angle, 120°bond spacing, 18% of widthfixed length, 14.4 pt (0.508 cm, 0.2 in.)bold width, 2.0 pt (0.071 cm, 0.0278 in.)line width, 0.6 pt (0.021 cm, 0.0084 in.)margin width, 1.6 pt (0.056 cm, 0.0222 in.)hash spacing, 2.5 pt (0.088 cm, 0.0347 in.)
- As text settings, select: font, Arial/Helveticasize, 10 pt
- Under the preferences, choose: units, pointstolerances, 5 pixels
- Under page setup, choose: paper, US Letterscale, 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.

### **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, to the same or additional reviewers, at the discretion of the 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.

## **Supporting Information**

This information is provided to the reviewers during the peer-review process (for Review Only) and is available to readers of the published work (for Publication). Supporting Information must be submitted at the same time as the manuscript. See the list of <u>Acceptable Software by File</u> <u>Designation</u> and confirm that your Supporting Information is viewable.

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Examples of sufficient descriptions: "Supporting Information: <sup>1</sup>H NMR spectra for all compounds (PDF)" or "Additional experimental details, materials, and methods, including photographs of experimental setup (DOC)".

Examples of insufficient descriptions: "Supporting Information: Figures S1-S3" or "Additional figures as mentioned in the text".

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# **Research Data Policy**

All ACS journals strongly encourage authors to make the research data underlying their articles publicly available at the time of publication.

Research data is defined as materials and information used in the experiments that enable the validation of the conclusions drawn in the article, including primary data produced by the authors for the study being reported, secondary data reused or analyzed by the authors for the study, and any other materials necessary to reproduce or replicate the results.

The <u>ACS Research Data Policy</u> provides additional information on Data Availability Statements, Data Citation, and Data Repositories.

## **Data Requirements**

**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., <sup>1</sup>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 spectrometric, 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 (**<sup>1</sup>**H NMR or** <sup>13</sup>**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 (or) 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, CCl4): 1.22 (t, 3, J = 7 Hz, CH2<u>CH</u>3), 2.58 (s, 1, OH), 3.70 (qd, 2, J = 7 Hz, OC<u>H</u>2CH3).

**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, <sup>1</sup>H and <sup>13</sup>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 g/kg, 1–10 g/kg, and 10–100 g/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*, 2<sup>nd</sup> ed. (Agricultural Handbook 436; U.S. Government Printing Office: Washington, DC, 1999) (available on-line at <a href="http://www.nrcs.usda.gov/wps/portal/nrcs/main/soils/survey/class/taxonomy">http://www.nrcs.usda.gov/wps/portal/nrcs/main/soils/survey/class/taxonomy</a>). 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, 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 <a href="http://www.aphis.usda.gov/animal\_welfare/links.shtml">http://www.aphis.usda.gov/animal\_welfare/links.shtml</a>. 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 <a href="http://www.cioms.ch/publications/guidelines/1985">http://www.cioms.ch/publications/guidelines/1985</a> 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 <a href="http://www.hhs.gov/ohrp/">http://www.hhs.gov/ohrp/</a>. 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.

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- there is evidence that the findings are unreliable but the authors' institution will not investigate the case;
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# **Appendix 2: Preparing Graphics**

### Resolution

Digital graphics pasted into manuscripts should have the following minimum resolutions:

- Black and white line art, 1200 dpi
- Grayscale art, 600 dpi
- Color art, 300 dpi

#### Size

Graphics must fit a one- or two-column format. Single-column graphics can be sized up to 240 points wide (3.33 in.) and double-column graphics must be sized between 300 and 504 points

(4.167 in. and 7 in.). The maximum depth for all graphics is 660 points (9.167 in.) including the caption (allow 12 pts. For each line of caption text). Lettering should be no smaller than 4.5 points in the final published format. The text should be legible when the graphic is viewed full-size. Helvetica or Arial fonts work well for lettering. Lines should be no thinner than 0.5 point.

### Color

Color may be used to enhance the clarity of complex structures, figures, spectra, and schemes, etc., and color reproduction of graphics is provided at no additional cost to the author. Graphics intended to appear in black and white or grayscale should not be submitted in color.

## **Type of Graphics**

## **Table of Contents (TOC)/Abstract Graphic**

Consult the Guidelines for Table of Contents/Abstract Graphics for specifications.

Our team of subject-matter experts and graphical designers can also help generate a compelling TOC graphic to convey your key findings. Learn more about our Graphical Abstract service.

## **Figures**

A caption giving the figure number and a brief description must be included below each figure. The caption should be understandable without reference to the text. It is preferable to place any key to symbols used in the artwork itself, not in the caption. Ensure that any symbols and abbreviations used in the text agree with those in the artwork.

#### Charts

Charts (groups of structures that do not show reactions) may have a brief caption describing their contents.

### **Tables**

Each table must have a brief (one phrase or sentence) title that describes the contents. The title should be understandable without reference to the text. Details should be put in footnotes, not in the title. Tables should be used when the data cannot be presented clearly in the narrative, when many numbers must be presented, or when more meaningful inter-relationships can be conveyed by the tabular format. Tables should supplement, not duplicate, information presented in the text and figures. Tables should be simple and concise.

### **Schemes**

Each scheme (sequences of reactions) may have a brief caption describing its contents.

#### **Chemical Structures**

Chemical structures should be produced with the use of a drawing program such as ChemDraw.

#### **Cover Art**

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