

Last updated: October 29, 2024 [View the latest guidelines online](#)

Scope of the Journal

The Journal of Organic Chemistry (JOC) welcomes original contributions of fundamental research in all branches of the theory and practice of organic chemistry. In selecting manuscripts for publication, the editors place emphasis on the quality and novelty of the work, as well as the breadth of interest to the organic chemistry community.

Manuscripts with a focus on the following topics along with guidance are included below. The scope of organic chemistry is broader than these several areas of research and the Editorial Board is consistently welcoming and evaluating manuscripts addressing topics in addition to these. Guidelines for specific focus areas are as follows:

- (a) Single or multistep synthetic methods manuscripts and total synthesis manuscripts are expected to demonstrate strategies, transformations, or shortened routes to target structures that show conceptual novelty, not merely the extension of previously reported chemistry to a different class of reaction substrates, reagents, or catalysts.
- (b) Manuscripts focusing on mechanistic studies (experimental or theoretical) should show methodological advances or provide novel insight into the course of chemical reactions, rather than only confirming previously established mechanisms.
- (c) Natural products isolation and identification studies should report unusual skeletal features, improvements in methods for structural determination, or insights into biosynthetic pathways.
- (d) Manuscripts with elements of biological study, analytical chemistry, functional molecules and systems, or materials science should demonstrate novelty in those aspects associated with the organic chemistry portion of the work being reported.

If you are a new JOC author, or if you have not submitted a manuscript during the past year, please read and familiarize yourself with these complete Author Guidelines to ensure you are up to date with all of the journal's manuscript preparation and submission requirements.

Editors, Authors, and Reviewers should read the [ACS Ethical Guidelines](#).

Emphasis on Chemical Safety

In 2021, in support of ACS's core value of "Professionalism, Safety, and Ethics," ACS Publications added a Safety Considerations requirement to the Author Guidelines of every ACS journal (Appendix 1):

Authors must emphasize any unexpected, new, and/or significant hazards or risks associated with the reported work. This information should be in the Experimental Section of a full article and included in the main text of a letter. Statement examples can be found in the [Safety Statement Style Sheet](#) and additional information on communicating safety information from the *ACS Guide to Scholarly Communication* [is freely available here](#).

The Journal of Organic Chemistry is participating in a pilot program to further encourage use of Safety Statements in manuscripts, including details on how to mitigate hazards and risks. Reviewers and Editors will be more carefully checking manuscripts to determine whether an

existing Safety Statement is accurate and complete, and if there is no Safety Statement in a manuscript whether there are any hazards or risks that require a Safety Statement be added. If a Safety Statement is needed, authors will be asked to include one in their manuscript at revision and before acceptance.

Manuscript Types

Articles are comprehensive, critical accounts of the solution of significant problems. Articles based on work reported in a preliminary letter or communication are welcome and encouraged, *provided they represent a substantial amplification and extension of the earlier work*, not merely the addition of experimental details or further examples. Such submissions may include new experimental procedures, additional data, significantly expanded discussion, and further conclusions. Results reported in the preliminary publication may be included when the author believes readers will benefit from having all the related data collected in a single paper. The letter or communication must be mentioned in the cover letter and cited in the manuscript's introductory remarks. For the convenience of the reviewers and editor, a copy of the preliminary report and any associated supporting information must be furnished as supporting information for review only.

Featured Articles are submitted Articles selected by the editors for their quality, interest, and importance, and have also received especially strong positive comments from reviewers. These articles receive expedited processing during journal production and appear at the beginning of the Articles section of each issue. They are also highlighted in a [special section on the Journal's website](#).

Notes are concise accounts describing novel observations, new methods of wide applicability or interest, or focused studies of general interest. Notes differ from Articles in having a narrower scope. The level of experimental rigor, including compound characterization, required for a Note is the same as that for an Article. The length of a Note is limited to 3,000 words, which includes the abstract, introductory paragraph, results and discussion, and space occupied by tables and graphics; the word count limit does not include the experimental section, acknowledgments, supporting information availability statement, and list of references. Tables and graphics count toward the word-count limits at the rate of 50 words per vertical inch for one-column items (8.4 cm/3.3 inches wide or less), and 100 words per vertical inch for wider items up to two-columns (17.8 cm/7.0 inches). Authors are reminded that any graphics that are reduced in size to help adhere to the above length limits need to be fully legible when the page is printed at 100% scale.

JOCSynopses are brief focused reviews of current topics of interest to organic chemists written by active researchers that include work from their own laboratories. Manuscripts that describe newly emerging areas of research are encouraged. JOCSynopses are invited by the Editor-in-Chief but voluntary submissions will be considered and screened before a formal review. They are limited to 4,000 words of text, not counting acknowledgments and the list of references, and are limited to no more than 80 references and endnotes. All graphics and tables combined must be able to fit on two standard word-processor pages. Authors are reminded that any graphics that are reduced in size to help adhere to the above length limits need to be fully legible when the page is printed at 100% scale.

Perspectives are personal overviews of specialized research areas by acknowledged experts. They are published only by invitation of the Editor-in-Chief. Details on length and other requirements will be provided to authors.

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 [ACS Researcher Resources](#) 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 the ACS Publications manuscript submission and peer review system, including details on selecting the applicable [Journal Publishing Agreement](#).
- [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 [here](#).

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 templates facilitate the peer review process by allowing authors to place artwork and tables close to the point where they are discussed within the text. Learn more about document templates [here](#).

General information on the preparation of manuscripts may also be found in the [ACS Guide to Scholarly Communication](#).

Acceptable Software, File Designations, and TeX/LaTeX

See the list of [Acceptable Software](#) and appropriate [File Designations](#) to be sure your file types are compatible with the submission system. Information for manuscripts generated from [TeX/LaTeX](#) 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.

The cover letter should include a brief paragraph pointing out the significance of the reported work. Information regarding previous submission to *The Journal of Organic Chemistry* or to any other ACS journal should be included.

Manuscript Text Components

In general, manuscripts must contain: (1) Title, (2) Authors' names and addresses, (3) Corresponding author's email address, (4) Table of Contents/Graphic, (5) Abstract, (6) Introduction, (7) Results and Discussion [may be separate], (8) Conclusion [optional], (9) Experimental Section and/or Computational Methods [except Perspectives, *JOC*Synopses], (10) Acknowledgments [optional], (11) Data Availability Statement, (12) Supporting Information availability statement [required if the manuscript is accompanied by any supporting information for publication], and (13) References and Endnotes. The order of these components is recommended as shown, but we give authors flexibility to change the order of items 7-9 to best fit their manuscript.

Claims of priority, originality, convenience, effectiveness, or value should be avoided or used with great restraint. For example, the words "convenient", "efficient", "elegant", "expedient", "facile", "first", "new", "novel", "practical", "simple", "unique", "unprecedented", and "versatile" should not be used. The use of "free" should also be avoided, that is "metal-free," "catalyst-free," "light-free," and so on, as these terms can be misleading. In addition, editors may ask authors to moderate or remove what they judge to be excessive use of subjective evaluative language elsewhere in the manuscript.

Section Headings. The only section headings used in a Note are **Experimental Section**, **Computational Methods** (if needed), **Supporting Information**, **Acknowledgments**, and **References**. An Article has **Introduction**, **Results and Discussion**, **Conclusion** (optional), **Experimental Section**, **Computational Methods** (if needed), **Supporting Information**, **Acknowledgments**, and **References**. A *JOC*Synopsis has the same section headings as a Note, except that there is no Experimental Section/Computational Methods.

Title. The title should be descriptive of the topic of the article and as short as possible, using easily searchable keywords and minimizing hyphenation. Avoid using abbreviations and acronyms unless they are more commonly used than spelled out words. Also avoid complex compound names as much as possible in the title by using generic names, and spell out elements rather than using symbols unless part of a compound name. Neither the title nor any other text should indicate that the article is part of a numbered series on a broader research topic, or a numbered contribution from a particular institution or research group.

Abbreviations, Symbols, Units, Compound Names. Authors should use abbreviations and

acronyms in the text to conserve space. A [list of standard abbreviations](#) is provided in the ACS Guide to Scholarly Publishing. Nonstandard abbreviations and acronyms must be defined the first time they are used in the abstract, text, and supporting information. The use of abbreviations should be consistent throughout the manuscript text and graphics. For example, either CH₃ or Me may be used for “methyl,” but not both. Full systematic names of compounds (see Part 4 and Part 5 of [the ACS Guide to Scholarly Communication](#) for guidance) should be included in the Experimental Section on first mention and for brevity assigned a molecule number for reference throughout the article. In other sections of the manuscript, authors should use their judgement on common usage of compound names or use a generic name or molecule numbers in lieu of full systematic names. As a courtesy to the research community, a list of abbreviations used in your manuscript if extensive can be included under Associated Content at the end of the manuscript and at the end of the Supporting Information before the References section.

Abstract. The abstract for an Article or Note should briefly state the purpose of the research, principal results, and major conclusions. A well-written abstract can attract the attention of potential readers and increase the likelihood that the published article will be cited by other researchers. Summaries of numerical results should be quantitative (for example, “in yields of 65 to 90%” rather than “in good to excellent yields”). Undefined nonstandard abbreviations and reference citation numbers should be avoided. For a *JOCSynopsis* or Perspective, the abstract should identify the scope and focus of the manuscript.

The length of the abstract for an Article or Perspective should not exceed 200 words. The length of the abstract for a Note or *JOCSynopsis* is limited to 80 words.

Abstract/Table of Contents Graphic. See Appendix 2 for full details on graphics requirements. A graphic must be included with each manuscript for display in the Abstract and Table of Contents (TOC), fitting in an area no larger than 8.25 cm by 4.45 cm (3.25 inches by 1.75 inches). This graphic should capture the reader’s attention and, in conjunction with the title, should give the reader a quick visual impression of the essence of the article. In preparing a TOC graphic, creativity is welcome, but avoid images of people living or from the past and avoid caricatures or parodies that could be socially/culturally insensitive or considered racist or discriminatory, especially when taken out of context. Ensure that cartoon depictions of machinery, nature, and processes do not indicate actions or settings that are improbable.

Introduction. The introduction should include sufficient background information to provide appropriate context as to the novelty and importance of the new work and clearly state the purpose and objectives of the research. An extensive review of prior work is not appropriate, and documentation of the relevant background literature should be selective rather than exhaustive, particularly if reviews can be cited. The opening paragraph of a Note or *JOCSynopsis* serves a similar function but is briefer and is not labeled as an **Introduction** section.

Results and Discussion. The presentation of experimental details in the results and discussion section should be kept to a minimum. Reiteration of information that is made obvious in tables, figures, or reaction schemes should be avoided. A **Results and Discussion** section heading is used in an Article but not in a Note or *JOCSynopsis*.

Conclusion. If an optional conclusion section is provided, its content should not substantially duplicate the abstract.

Experimental Section/Computational Methods. For Notes and Articles, manuscripts reporting the results of experimental work must include *all* experimental procedures, compound

characterization data, and any associated literature citations. **Authors have the flexibility to place the experimental content in the main text (Experimental Section), in the Supporting Information, or a combination of both as it best supports the manuscript, so long as the information is accurate and complete.** As needed, authors may substitute or also include a section on Computational Methods. These sections should describe methods in sufficient detail to permit repetition of the work by others. [The Data Requirements section](#) should be consulted for guidance on reporting synthetic experimental, compound characterization, spectroscopic, crystallographic, computational, and bioassay data in the Experimental Section, Computational Methods, and Supporting Information. A general Experimental Methods paragraph may be optionally provided to document procedures, such as purification methods, solvent removal, and spectroscopic and chromatographic analyses, that are common to most of the individual procedures, and should be placed at the beginning of the Experimental Section.

Please organize your Experimental Section as follows:

- General Section
- Synthesis of starting materials
- Tabulated data for starting materials (if new compounds)
- Typical procedure for products
- Tabulated data for products

Please organize your Supporting Information in this order:

- Table of Contents (with page numbers)
- SI Table(s)
- ^1H and ^{13}C NMR data
- DFT calculations

Data Availability Statement. A Data Availability Statement is required for all peer-reviewed articles and is not required for the following non-peer-reviewed articles: Addition/Correction, Editorial, Expression of Concern, or Retraction. The [ACS Research Data Policy](#) provides additional information on [Data Availability Statements](#), Data Citation, and Data Repositories.

References. Authors should be judicious in citing the literature; unnecessarily long lists of references should be avoided. If a number of publications are relevant to a statement in the text, not more than two or three of the most seminal or recent should be cited; if appropriate, the author may add “and references cited therein” following a reference. Authors must also cite any previously published work wherein portions of the submitted work have been disclosed. It is seldom necessary or appropriate for an author to cite more than 10 of their own publications, except in a Perspective or *JOCSynopsis*. No reference should repeat a reference that appears elsewhere in the manuscript’s list of references. Authors are encouraged to include additional references cited in Supporting Information files in the main article reference list. Long endnotes should be avoided; peripheral discussion should be placed in the supporting information. Endnotes should not contain graphics, experimental procedures, or compound characterization data.

Author portrait for Perspectives and JOCSynopses. A high-resolution (300 dpi or better), in focus, color head-and-shoulders photograph of each coauthor or a group photo of the team and a brief one or two sentence statement of current research interests should be included in the Author Information section. Model release and copyright forms are required for author photographs and will be provided by the Journal office.

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 [Acceptable Software by File Designation](#) and confirm that your Supporting Information is [viewable](#).

If the manuscript is accompanied by any supporting information files for publication, these files will be made available free of charge to readers. A brief, nonsentence description of the actual contents of each file, including the file type extension, is required. This description should be labeled Supporting Information and should appear before the Acknowledgement and Reference sections. Examples of sufficient and insufficient descriptions are as follows:

Examples of sufficient descriptions: “Supporting Information: ^1H 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”.

When including supporting information for review only, include copies of references that are unpublished or in-press. These files are available only to editors and reviewers.

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 [ACS Research Data Policy](#) provides additional information on Data Availability Statements, Data Citation, and Data Repositories.

Data Requirements

For Notes and Articles, every manuscript reporting the results of experimental work must include an Experimental Section, with *all* experimental procedures, compound characterization data, and any associated literature citations appearing in the manuscript: Authors may use their discretion to place the information in the main text or in the Supporting Information, depending on the relevance to the Results and Discussion section. The Experimental Section should describe methods in sufficient detail to permit repetition of the work by others. The section below on “Specialized Data” should be consulted for guidance on reporting synthetic experimental, compound characterization, spectroscopic, crystallographic, computational, and bioassay data in the Experimental Section and Supporting Information. The editors remind authors that it is unethical to modify reported data or spectra, for example to correct spectral baselines or remove solvent or impurity peaks.

General Experimental Methods. A General Experimental Methods paragraph may be optionally provided to document procedures (such as purification methods, solvent removal, and spectroscopic and chromatographic analyses) that are common to most of the individual procedures, and it should be placed at the beginning of the Experimental Section. Sources of stationary phases for chromatography and supports for solidphase synthesis may be

identified. Sources of reactants, reagents, and solvents should *not* be identified except for (1) starting compounds that are unusual or not widely available; (2) materials for which the author has reason to suspect that the source is critical to the outcome of an experiment; and (3) catalysts. In the latter two cases, available purity information should be reported. Experiments involving a catalyst, enzyme, or reagent that is neither commercially available nor prepared by a fully described or cited nonproprietary method may not be reported.

Specialized Data.

All data needed to document structure assignments, purity assessments, and other conclusions should be included in the manuscript and Supporting Information.

Synthesis Experiments. Synthesis procedures for new compounds should be accompanied by yields and the most important product characterization data. Graphic structures of synthesized products (but not reaction schemes or other graphics) may accompany the characterization data listings. When known compounds have been prepared, procedures that were reported in the Experimental Section or Supporting Information of a previous publication should be cited but not reported in detail unless they have been modified.

Fully characterized compounds should have bolded compound names and structure numbers as the titles of the paragraphs in which their preparation, isolation, purification, and properties are described. Intermediates in multistep sequences that have not been purified and fully characterized should not have their names bolded; their preparation and partial characterization should be described as a step in the synthesis of a fully characterized bold-titled compound.

Reactant, reagent, and catalyst quantities should be given in both weight and molar units. Reaction solvent volumes and reaction times should be reported. Use of standard abbreviations or unambiguous molecular formulas for reagents and solvents, and of structure numbers rather than chemical names to identify starting materials and intermediates, is encouraged.

All reported yields should represent weighed amounts of isolated and purified products and must be reported in the Experimental Section as both weights and percentages. The Editors would like to point out that reported yields above 95%, isomer ratios above 200:1, and enantiomeric excesses above 99% typically aren't realistic without further explanation. When a series of related compounds has been prepared using substantially the same procedure, it is usually sufficient to present a single representative example. If instead a general synthesis procedure reporting only relative molar quantities (as equivalents) is presented, the relative solvent volume also needs to be reported (as the molarity of the limiting reactant or reagent in the reaction mixture). If the several examples were not all conducted at the same molar scale, the paragraphs describing the individual products should include, along with the yields, the weights and molar amounts of the limiting reactants, for example, "yield 177 mg (78%) from 198 mg (0.66 mmol) of 3d."

When chromatographically or spectroscopically determined conversions of starting material to product are presented in a table documenting a synthetic transformation using a range of starting materials, reagents, or reaction conditions, a column heading or footnote should identify which quantity is being reported. The isolation and purification of the products for several representative examples should be reported in the Experimental Section, and the yields of isolated product for those examples should be included in the table.

Manuscripts that illustrate a new or modified synthetic method with multiple examples conducted on a submillimolar scale should include one or more examples carried out on a larger scale (1 mmol) to demonstrate the practical utility of the method as a synthetic tool; exceptions may be discussed with the editor for certain materials chemistry and electrochemistry work.

When preparative chromatography is used for product purification, both the stationary phase and solvent should be identified. Where different solvent mixture ratios, or different gradient elution schemes, have been used for purifying the members of a series of related compounds whose preparation is described with a single example or a single general procedure, the mixture

composition or gradient scheme should be individually reported for each compound.

For reactions that require heating, identify the temperature and heat source (oil bath, heating mantle, etc.) or the model and manufacturer number if a device is used, e.g. a microwave or sonicator. Reports of syntheses conducted in microwave reactors must indicate whether sealed or open reaction vessels were used, how the reaction temperature was monitored (external surface sensor or internal probe type), and the temperature reached or maintained in each experiment. Authors must comply with the requirement that at least one detailed complete method must be provided at the 1 mmol scale. *JOC* does not publish reports of studies conducted with domestic (kitchen) microwave ovens in which yields or selectivities observed using microwave irradiation are compared with results obtained using conventional heating.

For light-promoted reactions, report the light source: type of lamp along with manufacturer and model or type of lights, wavelength of peak intensity or broadband source, and available information about the spectral distribution and intensity; the identity and quantity or concentration of any photocatalyst or sensitizer; the material of the irradiation vessel if other than borosilicate glass; the distance from the light source to the irradiation vessel; and the use of any filters.

In addition to emphasizing safety hazards or risks associated with the reported work and how to mitigate them, the Editors encourage authors to include comments on the use of toxic and/or environmentally persistent reagents and solvents and provide a rationale on choice of these reagents and solvents. This acknowledgement is especially important in cases of “dual use” potential when the reported work could be directly misapplied by others to pose a threat to public health and safety. *JOC* further encourages authors to consider the Principles of Green Chemistry in carrying out their research and consider reporting metrics such as atom economy, mass efficiency, E-factor, or others. For more information, please consult [Research Tools](#) provided by the ACS Green Chemistry Institute.

Compound Characterization Data.

JOC upholds a high standard for compound characterization to ensure that compounds being added to the chemical literature have been correctly identified and can be synthesized in reported yield and purity. For new compounds, evidence adequate to establish both *identity* and *degree of purity* (homogeneity) must be provided. Purity documentation must also be provided for known compounds whose preparation by a new or modified literature method is reported. *JOC* requires that purity be documented compound-by-compound, with copies of spectra or chromatograms, elemental analysis, or quantitative NMR or chromatographic integration data. For combinatorial libraries containing more than 20 new compounds, complete characterization data must be provided for at least 20 diverse members of each structural type. Full characterization is not required for new compounds prepared solely as derivatives for analytical purposes (for example, Mosher esters prepared for assigning absolute configuration). Authors are further encouraged to include additional data or revised data that was not reported in original references cited, and in doing so indicate which part of the data set is new information.

Authors are responsible for retaining their original data or having available original data from collaborators or from contractors who perform analyses on their behalf. Authors may be asked to provide copies of spectra or analytical reports if an editor or reviewer raises a question about reported results. Upon publication, authors are encouraged to link the manuscript to their data housed in a repository or other location, and to make their primary data freely available to others upon request.

JOC provides a [Compound Characterization Checklist](#) for authors to use when reporting new compounds or when reporting known compounds that have been prepared by new or modified methods. Known compounds that have been synthesized by literature methods or obtained from commercial sources should not be listed, but appropriate references or sources should be cited in the manuscript. The Checklist, which was previously required, is now optional, as the editors recognize enhanced efficiencies in data reporting and *JOC* has a rigorous data-checking process as part of manuscript evaluation. Nevertheless, authors are highly encouraged to use the checklist

for their own benefit and to help editors and reviewers more quickly assess the thoroughness of the characterization of compounds and the reporting of computational results. The Compound Characterization Checklist will not be published.

If required data cannot be obtained (a compound is too insoluble to record a carbon NMR, or too unstable to obtain a good elemental analysis, etc.), the reason for the absence of the data should be noted in the Experimental Section to avoid having review held up by a journal office request for the missing data.

When the preparation of known compounds *by a new or modified method* is reported, it is only necessary to report the yields, cite the published characterization data, and document the purity, usually by inclusion of proton NMR spectra or chromatograms in the Supporting Information (see section on Purity below). It is not necessary to include detailed NMR, IR, and MS peak listings in either the Experimental Section or Supporting Information unless erroneous data in the literature are being corrected, or unless the data are being reported for the first time.

For known compounds synthesized *by published methods* as reactants, reagents, catalysts, or study materials for physical or biochemical investigations, the literature data that were compared with the measured spectroscopic and physical data to confirm the materials' identity should be cited. Detailed synthesis procedures and listings of characterization data should not be included for these compounds unless the literature procedure has been substantially modified, or new physical or spectroscopic data are being presented.

Mixtures of regioisomers, geometric isomers, and diastereomers (but not usually enantiomers) are generally expected to be separated, and the components individually characterized. When the components cannot be successfully separated and the individual gravimetric yields determined, the combined yield and the mole fraction of each component should be reported in the Experimental Section, and the spectroscopic or chromatographic method by which the composition was determined should be identified.

All compound preparation procedures and characterization data should be included in the manuscript, but at the authors' discretion may appear in the Experimental Section or in the Supporting Information, so long as the information is accurate and complete. The formatting of spectroscopic, physical, analytical, and other product characterization data should adhere to the recommendations in [the ACS Guide to Scholarly Communication](#), except that NMR and accurate mass (HRMS) data should be reported as discussed below. For compounds that have been prepared by more than one method, the description in the Experimental Section and the purity documentation (usually a proton NMR spectrum in the Supporting Information) should clearly identify which method provided the sample whose yield and purity are documented.

Identity.

Evidence for documenting the identity of new compounds should include **both** proton and carbon NMR data **and either** MS accurate mass (HRMS) **or** elemental analysis data. Where other types of physical and spectroscopic methods are useful or necessary for confirming structure assignments, it is appropriate to include a summary of the data in the Experimental Section, but except as noted below, these additional data types are not generally required for routine compound characterization in *JOC*. Such data types include IR, UV-visible, low resolution MS, GCMS, LCMS, 2D NMR (except where peak assignments are reported), and X-ray crystallography.

NMR (see also the section on Computational Data below). Proton and carbon NMR resonances should be listed for each new compound, with the normal full range of chemical shifts displayed (usually 10–0 ppm for proton; 200–0 ppm for carbon); the solvent and instrument frequency should be identified. The use of broadband decoupling should be indicated with braces, for example $^{13}\text{C}\{^1\text{H}\}$ for proton-decoupled carbon data. Proton NMR shifts, reported to 0.01 ppm precision, should be accompanied by an abbreviation for any multiplet structure, the number of atoms

represented by the peak or multiplet, and coupling constants where applicable. Carbon NMR peak shifts should be rounded off to the nearest 0.1 ppm except when greater precision is needed to distinguish closely spaced peaks. Information about numbers of attached hydrogen atoms (reported as C, CH, CH₂, CH₃) from DEPT, DEPTQ, PENDANT, or 2D spectra may be included with the carbon peak shifts. For compounds with carbon-bonded fluorine atoms, the carbon peak multiplicity (d, t, q) and coupling in Hz should be reported.

A typical example to report ¹H and ¹³C NMR data to conform to *the ACS Guide to Scholarly Communication* format is (high to low): ¹H NMR (C₆D₆, 400 MHz): 6.00 (t, 1H, J = 4.0 Hz), 5.62 (t, 1H, J = 4.0 Hz), 1.95 (d, 1H, J = 4.0 Hz), 1.73 (s, 15H), 1.62 (s, 3H), 1.58 (s, 15H), 0.98 (s, 1H), 0.72 (d, 1H, J = 4.0 Hz), -0.53 (s, 1H). ¹³C{¹H} NMR (C₆D₆, 125 MHz): 88.7, 88.0, 81.0, 80.8, 60.6, 54.2, 51.5, 38.3, 17.4, 10.6, 10.2.

Detailed peak assignments (including "ArH" for aromatic protons and "C=O" for carbonyl carbons) should *not* be reported in the Experimental Section unless one or more 2D methods have been used to establish atom connectivities and spatial relationships, and the type(s) of 2D methods are identified in a General Experimental Methods paragraph or in the individual compound data listings. Authors using software for automated data analysis are reminded to check numerical data, including proton counts and coupling constants, before including them in the manuscript. For products isolated as inseparable isomer mixtures, if the NMR absorptions can be attributed to individual isomers, the NMR chemical shift data for those isomers should be reported in two or more separate lists, one for each isomer, instead of as a single list. For proton NMR data, the integrals in each isomer's list should be reported in whole numbers of protons.

For every new compound, a copy of a well-resolved 1D proton NMR spectrum and a copy of a proton-decoupled 1D carbon spectrum (conventional, DEPT, DEPTQ, or PENDANT), should be included in the supporting information. The proton spectra should include numerical integration data reported to 0.1 or 0.01 hydrogen atom precision; analog integration "steps" do not need to be displayed, and if shown they must not obscure the underlying absorption peaks and multiplets. The resolution of the spectra should be high enough so that multiplet fine structure can be examined by increasing the image magnification (zoom). In cases where structure assignments of complex molecules depend heavily on NMR data interpretation, including isolated and synthesized natural products, copies of the 2D spectra should also be furnished. Authors may also include with their spectra tables of NMR data containing assigned ¹³C and ¹H chemical shifts with signal multiplicities and couplings (if measured) and 2D NMR correlations so the data are more readily accessible.

For enantioenriched or isotopically labeled forms of compounds whose racemic or unlabeled forms are known (or are fully characterized in the same manuscript), listings of NMR chemical shift data are not required, but either copies of NMR spectra, chromatograms, or other data are needed to document the chemical purity.

One of the purposes of including copies of NMR spectra in the Supporting Information is to qualitatively demonstrate the purity of the materials obtained when the reported reaction, isolation, and purification methods are used. It is not acceptable to use peak-editing software or other means to suppress or obscure peaks arising from impurities (including byproducts, unconsumed reactants, and incompletely removed extraction, chromatography, or recrystallization solvents). Peak suppression may be used on the NMR solvent peak for samples run in protic solvents, but it is never necessary for samples run in deuterated solvents.

Primary NMR Data Files.

Authors are requested to furnish primary NMR data files (FID files, acquisition data, processing parameters). All original primary NMR data supporting a submission should be retained and provided if requested. For more information on packaging primary NMR data and metadata for

submission, see the [ACS Research Data Center](#).

When submitting FID files:

- One folder should be created for each compound
- Folder should be named clearly, using the compound number
- Include the FID files, acquisition data and processing parameters for each experiment
- Name each spectrum according to the type of nucleus measured: ¹H, ¹³C, DEPT, COSY, etc.
- NMR files should be compressed into zip file(s)
- Name the zipped file, "FID for Publication."

In a text document, include the name of the manufacturer of the spectrometer used to collect the data, the acquisition software and processing programs used to analyze the data, and the field strength used to measure each nucleus (i.e., 300 MHz ¹H or 50 MHz ¹³C). Include a structure file that shows the structure and compound identifier for each provided dataset. MolFile is the recommended format and is strongly preferred.

Elemental Analysis and Accurate Mass Measurement. For most new compounds except large molecules (> 1000 m/z), polymers, and biomacromolecules (see below), either combustion elemental analysis or mass-spectrometric accurate mass (high-resolution mass spectrometry [HRMS] or "exact mass") data should be reported to support the molecular formula assignment. The data should be reported in [the ACS Guide to Scholarly Communication](#) format and should include the molecular formulas on which the theoretical (Calcd) values are based.

When the scope of a new or modified synthetic method is illustrated with multiple examples, the description of each reactant or product that is a new compound needs to include elemental analysis or HRMS data. However, see above regarding journal's requirement when large combinatorial libraries are being characterized.

In reporting compounds prepared by linear, branched, or convergent multistep sequences, the characterization of at least every third compound needs to include elemental analysis or HRMS data. A new compound that is a branching point, a convergence point, or the final new compound in a synthetic scheme, needs elemental analysis or HRMS data regardless of whether the precursor or successor compounds are fully characterized or previously reported. A new compound that lacks elemental analysis or HRMS data should not have its name bolded in the experimental section; instead, it should be described as an intermediate in the synthesis of the next fully characterized, bold-titled compound.

When a diastereomer or regiosomer mixture cannot be separated into its components, it is usually expected that elemental analysis or HRMS data will be reported for the mixture. Elemental analysis or HRMS data are not required for enantioenriched versions of compounds characterized as racemates in the same article or in the literature, or for the second enantiomer when the synthesis and isolation of both enantiomers is reported. In these cases, the chemical and enantiomeric purities of each enantiomer will need to be documented. Such enantiomers should have "racemate known" or "opposite enantiomer known" entered on the [Compound Characterization Checklist](#) to avoid a Journal office request for elemental analysis or HRMS data. Elemental analysis or HRMS data are not required for isotope-labeled versions of compounds already known in their unlabeled form unless such data are needed to demonstrate the extent of the labeling. A HRMS measurement is more useful than elemental analysis data when a transformation causes only a small change in the atomic composition (for example, hydrogenation of a carbon-carbon bond in a large molecule).

[The ACS Guide to Scholarly Communication](#) format for reporting elemental analysis data is: Anal. Calcd for C₁₃H₁₇NO₃: C, 66.36; H, 7.28; N, 5.95. Found: C, 66.55; H, 7.01; N, 6.22. Elemental analysis Found values for carbon, hydrogen, and nitrogen should be within 0.4% of the Calcd values for the proposed formula. The need to include fractional molecules of solvent or water in

the molecular formula to improve the fit of the data usually reflects incomplete purification of the sample. In such cases, either a portion of the product should be repurified and reanalyzed, or HRMS data should be obtained. If any of the reported formulas include solvent or water, independent evidence for its presence needs to be reported immediately following the Found values.

Accurate mass measurements should be performed at a mass resolution sufficient to minimize interferences. The reported molecular formulas and Calcd values should include any added atoms (usually H or Na). The ionization method and mass analyzer type (for example, Q-TOF, magnetic sector, or ion trap) should be reported. [*The ACS Guide to Scholarly Communication*](#) format for reporting accurate mass data is: HRMS (ESI/Q-TOF) m/z : $[M + Na]^+$ Calcd for $C_{13}H_{17}NO_3Na$ 258.1101; Found 258.1074. The number of potential molecular formulas within a given mass range centered on a measured (Found) value increases rapidly with molecular mass. A Found value within 0.003 m/z unit of the Calcd value of a parent-derived ion, together with other available data (including knowledge of the elements present in reactants and reagents) is usually adequate for supporting a molecular formula for compounds with molecular masses below 1000 amu. Higher accuracy may be needed for compounds of higher mass, and for compounds of uncertain synthetic or biosynthetic origin, such as isolated natural products and their derivatives.

A single-crystal X-ray diffraction structure is generally an acceptable alternative to elemental analysis or HRMS data for confirming the molecular formula.

Configurational Isomer Mixtures. The composition of enantioenriched isomer mixtures and diastereomer mixtures, determined from NMR, chromatographic, or other data, should be reported. Either mole fractions, or enantiomer or diastereomer ratios, are preferred over enantiomeric or diastereomeric excess values. Copies of the spectra or chromatograms should be included in the supporting information.

Experimental Electronic Circular Dichroism and Vibrational Circular Dichroism Spectra.

Experimental conditions of ECD and VCD spectra such as concentration, solvent, and optical path length should be indicated. Spectral intensities should be reported in units of molar absorptivity ($M^{-1} cm^{-1}$). The method of baseline correction (subtraction of solvent or racemate spectrum) must be noted. The spectra should always be presented together with the corresponding unpolarized absorption spectra (UV/vis and IR) shown at the same scale. See also the section on Computational Data.

Oxygen Balance. Oxygen balance parameter gives potential of a compound or an explosive towards oxidation. Please report the oxygen balance in the following format including the complete formula used for calculation:

•Oxygen balance (OB, %) for $CaHbNcOd$: $OB = 1600 \times (d - 2a - b/2) / Mw$, Mw = molecular weight (based on carbon dioxide).

Specific Rotation. Specific optical rotations should be reported for isolated natural products and enantioenriched compounds when sufficient sample is available. Specific rotations based on the equation $[\alpha] = (100 \times \alpha) / (l \times c)$ should be reported as unitless numbers as in the following example: $[\alpha]_D^{20} -25$ (c 1.9, $CHCl_3$), where the concentration c is in g/100 mL and the path length l is in decimeters. The units of the specific rotation, $(deg \times mL) / (g \times dm)$, are implicit and are not included with the reported value. See also the section on Computational Data.

Physical State and Melting Point. The description of new compounds should include a statement of whether the isolated material is a crystalline solid, an amorphous solid, a gum, or a liquid. The color should be reported if it is not colorless or white. A melting point *range* should be reported for every **new** crystalline solid product. Melting point ranges may be reported to

document the purity of **known**, but not new, synthesis products (see below). Authors are encouraged to report melting point ranges for recrystallized samples of known compounds that were previously reported only in noncrystalline (and presumably less pure) form.

Infrared and Low-Resolution MS. If infrared and low-resolution mass spectrometric data are reported, only those IR absorptions diagnostic for major functional groups, and only those MS peaks used for structure assignment, should be included in the experimental section. If IR band frequencies are reported, they should be rounded to 1 cm¹ precision. Whether or not IR bands or low-resolution MS peaks are listed in the experimental section, copies of the spectra may be included in the supporting information.

Purity. When primarily synthetic work is reported, *JOC* does not require that a certain minimum level of purity be met for the reported compounds, but it does require that the purity level that has been attained be faithfully documented. When new or known synthesized compounds are the study materials for physical measurements or bioassays, a purity level of at least 95% needs to be documented. Evidence for documenting compound purity should include one or more of the following:

- A standard 1D proton NMR spectrum or protondecoupled carbon NMR spectrum showing at most trace peaks not attributable to the assigned structure. A copy of a spectrum with a signal-to-noise ratio sufficient to permit seeing peaks with 5% of the intensity of the strongest peak should be included in the supporting information. The normal full range of chemical shifts should be displayed (usually 0–10 ppm for proton; 0–200 ppm for carbon). For *new* compounds, copies of *both* proton and carbon NMR spectra are required.
- Combustion elemental analytical values for carbon and hydrogen (and nitrogen, if present) agreeing with calculated values within 0.4%.
- Quantitative NMR data using an internal standard and based on peak area ratios determined under conditions that assure complete relaxation.
- Quantitative gas chromatographic analytical data for distilled or vacuumtransferred samples, or quantitative HPLC analytical data for materials isolated by column chromatography or separation from a solid support. The stationary phase, solvent (HPLC), detector type, and percentage of total chromatogram integration represented by the product peak should be reported. Alternatively, a copy of the chromatogram may be included in the supporting information.
- Electrophoretic analytical data obtained under conditions that permit observing impurities present at the 5% level.
- For *known* solid compounds, a narrow melting point range that is in close agreement with a cited literature value.

The type of evidence appropriate for demonstrating a compound's purity will depend on the method of preparation, the compound's air and thermal stability, structure complexity, the nature of likely impurities, and the amount of sample available. A narrow melting point range is not sufficient by itself to document the purity of a new compound. MS accurate mass (HRMS) data may be used to support a molecular formula assignment but cannot serve to document compound purity.

Biomacromolecules. The structures of biomacromolecules may be established by providing evidence about sequence and mass. Sequences may be inferred from the experimental order of amino acid, saccharide, or nucleotide coupling, from known sequences of templates in enzymemediated syntheses, or through standard sequencing techniques. Typically, a sequence will be accompanied by MS data to establish the molecular mass. A copy of a chromatogram, electropherogram, or blot should be placed in the supporting information to document the homogeneity.

Spectra. Reproductions of spectra will be published in the results and discussion section only when concise numerical summaries are inadequate for the discussion. Articles with a focus on interpretation of spectra, and those in which band shape or fine structure needs to be illustrated, may qualify for this exception. When presentation of spectra is essential, only the pertinent sections, prepared as figures, should be included. Spectra used as adjuncts to the characterization of compounds should be included in the supporting information.

Crystallographic Data. Only data and graphics integral to the discussion should be included in the manuscript file. If the data are used solely for confirming compound identity or stereochemistry, a statement in the results and Discussion or Experimental Section that the assignment is supported by an X-ray crystallographic structure determination is usually sufficient.

All Crystallographic Information Files (CIFs), structure factor tables, and CheckCIF reports must be submitted to the Cambridge Crystallographic Data Centre (CCDC) prior to manuscript submission. See [Requirements for Depositing X-Ray Crystallographic Data](#) [PDF] for complete details on submission of CIFs and a list of file types accommodated by CCDC.

- Before being submitted to CCDC, CIFs should be checked using the free checkCIF data-validation utility on the [CIF Validation](#) site.
- Any reported syntax errors should be corrected. Authors are required to correct/defend/or respond to any A-level alerts. Comments may be inserted into the CIF file using a Validation Response Form or uploaded as a separate document as Supporting Information for Review Only.
- checkCIF output files (combined into one PDF file) should be uploaded at submission as Supporting Information for Review Only.
- Any subsequent revisions to the CIFs or structure factor tables should be deposited directly with the CCDC before resubmitting the manuscript in ACS Paragon Plus.

For structures refined anisotropically, a thermal ellipsoid plot may be included in the manuscript file if it is useful to support the discussion. Otherwise, thermal ellipsoid plots, preferably full-page size, should be furnished as a figure in the Supporting Information. When presenting such structures, the ellipsoid contour percent probability level should be reported in the caption. A brief text description of the sample preparation and crystal structure determination should be included, and a paragraph or single table summarizing the crystal parameters and refinement metrics should accompany the thermal ellipsoid plot in the supporting information. Multi-page tables of atom positions, bond lengths, and bond angles *are not needed*, because those data are included in the required CIF file (see above). If a crystallographic model reproduced or derived from a published structure is illustrated for discussion purposes, a footnote immediately below the figure should clearly cite the source.

Bioassay Data. Because *JOC*'s scope does not include development of new bioassay methods, it is expected that reported bioassay data be collected following a cited method, so that a detailed description of the test protocol is not required. Alterations to the test method should be clearly noted where the results are presented, and the modified protocol should be described in the supporting information. Regardless of whether a standard or modified method is used, the bioassay description should include the range of concentrations or dosages tested, the number of replicates run at each concentration or dosage, and the statistical treatment or criteria used for drawing conclusions from the data. The reported results should include data for one or more standard test materials whose response to the assay is well documented, and quantitative results should include the standard deviations or ranges of the responses. When new or known synthesized compounds are the study materials for bioassays, a minimum purity level of 95% must be documented, at least for those samples showing substantial activity. It is recommended that samples showing the highest activity be repurified and reassayed to demonstrate that the measured bioactivity is not an artifact of highly active impurities.

Electrochemistry Data. For reporting Voltammetry and Amperometry measurements, and for reporting Bulk Electrolysis procedures, please see the [ACS Electrochemistry Guidelines](#).

Biological Data. For reporting information on specimens, techniques, and data, please see the [ACS Biological Data Guidelines](#).

Computational Data.

When computational results are included in a manuscript, complete details of methods and results, reported in sufficient detail to allow other researchers to repeat the computations, should be included either within the article in a Computational Methods section or as Supporting Information. Graphics of computationally derived models that are not vital to the discussion should be placed in the Supporting Information. The level of theory, basis set, and relevant input parameters should be identified along with the specific program used. The data should include Z-matrices or Cartesian coordinates, grid size (for DFT calculations), and computed total energies of target or optimized structures. Where applicable, the number of imaginary frequencies should be reported to identify stable structures and transition states.

Description of specific programs and versions. If the author's own or a modified version of a commercially available program is used, it is required that the program/code/modification be made available to the scientific community (QCPE, publication in a computational journal, commercially, etc.). Policies in this regard are identical with those of several other ACS journals, as summarized in *J. Chem. Inf. Model.* **2006**, *46*, 937. A clear exposition of any nonstandard equations and algorithms used and, where feasible, tests of the codes in various limiting cases should also be provided.

Details of the computations. The computed molecular model should be described clearly, possibly with a ChemDraw figure. If the model is based on an experimentally known complex/reaction, any modifications (such as truncations) should be clearly described and justified. Final optimized coordinates and keywords are to be provided. For DFT computations, the choice of functional must be justified, or the validation of the functional provided. The choice of basis sets must be explicitly discussed, including any deviation from standard basis sets. Convergence criteria, integration parameters, active space definition in multireference calculations, and, for open-shell systems, the way in which spin states are handled should be mentioned explicitly. The exact definition of any applied numerical or symmetry constraint should be indicated.

Details of the computational results. When relevant to the results of the study, data such as absolute energies, gross orbital populations, atomic spin densities, etc., should be supplied. Where feasible, critical checkpoint/restart files should be saved and made available upon request.

Cartesian Coordinates. Cartesian coordinates of all molecules, intermediates, transition states, etc. that are part of the manuscript must be uploaded in a single file that is formatted for convenient viewing with widely available molecular modeling packages. The .xyz and .mol formats are accepted at this time. The .xyz format is the most basic and easily prepared from computational output.

The first line of the .xyz format file denotes the number of atoms in the molecule.

The second line of the file is a comments line, and should begin with a descriptive name of the molecule/structure consistent with the designation in the manuscript, and any other pertinent information selected by the author, such as total energy.

Next follow lines for each element in the molecule. Each line contains the element symbol followed by the x, y, and z coordinates in angstroms (Å) separated by spaces in free-field format (i.e. precise formatting not required). More information on the .xyz file format is available at <http://openbabel.sourceforge.net/wiki/XYZ>.

Multiple structures are placed directly end-to-end in the file.

The file name should have the extension ".xyz". A simple example with three molecules is shown below.

It is strongly recommended that authors view the structures in the file with a modeling program before uploading the file. The program **Mercury** (version 3.3 or later) is recommended for viewing and manipulating the multiple structures. The Cambridge Crystallographic Data Centre (CCDC) offers **Mercury** at no cost. Include the phrase “a text file of all computed molecule Cartesian coordinates in a format for convenient visualization” in the Supporting Information statement.

For additional guidance, see the [ACS Simulations, Machine Learning, Computational Data guidelines](#).

When computational prediction of spectral properties is used to establish identity of new compounds, the following guidelines will apply:

- *General*: The level of theory, basis set, and relevant input parameters used for optimization and the prediction of spectral properties should be indicated in all cases. It must be noted/justified when geometry optimization and property calculations are carried out at different levels of theory.
- *Conformational search*. A thorough conformational search should be performed for all molecules, except those with no rotatable bonds. The methods and results of the conformational search should be reported in detail.
- *Optimized conformers*. The optimized geometries of all the conformers actually used to calculate a property should be reported, along with their energies and number of imaginary frequencies (if conformers are more than five, only significantly populated conformers, that is those with a calculated Boltzmann weight larger than 5%, can be reported).
- *¹H and/or ¹³C NMR chemical shifts*. The scaling parameters used to calculate chemical shifts must be indicated. Calculated isotropic shielding values (before scaling to chemical shifts) for H and/or C atoms of all considered conformers should be reported. If possible, comparison with experimental chemical shifts should be accompanied by R², RMSD, or DP4+ values. Statistical methods can be used as well.
- *Electronic Circular Dichroism*. Parameters used to simulate the UV/Vis and ECD curves such as Gaussian band width and UV shift must be indicated. A qualitative comparison of the experimental and computed ECD spectra is generally sufficient. A comparison of the experimental and computed UV/Vis spectra should also be presented. Transition energies (or frequencies) and rotational strengths should be reported in tabular form for the significantly populated conformers. A figure with computed ECD curves of individual conformers is suggested, but not required. Any figure comparing the experimental and computed spectra should include both the UV and ECD spectra in the same figure; both sets of spectra should be shown in the same wavelength range.
- *Vibrational Circular Dichroism*. Parameters used to simulate the spectra such as the Lorentzian band width and the frequency scaling factor must be indicated. The presentation of the comparison of experimental and computed spectra should include both the IR and VCD spectra in the same figure; both sets of spectra should be shown in the same wavenumber range (e.g., 1800-900 cm⁻¹). A qualitative comparison between experimental and computed spectra is sufficient as long as convincing band correlations between major features in the experimental and computed spectra are indicated. Quantitative comparison can be made using similarity analysis algorithms which provide a degree of congruence between measured and calculated VCD spectra for the assigned enantiomer versus its opposite enantiomer. If VCD is used to distinguish diastereomers, a particular emphasis of the spectra comparison must be given to those signals that are used to differentiate the stereoisomers.
- *Optical rotation*. When computed optical rotation values are used to assign or to complement

the assignment of an absolute configuration, it must be ensured that the experimental value is not solvent dependent (at least two experimental values in a polar and a non-polar solvent must be provided). Ideally, the optical rotation is also measured and computed at different wavelength.

Language and Editing Services

A well-written paper helps share your results most clearly. ACS Publications' [English Editing Service](#) is designed to help scientists communicate their research effectively. Our subject-matter expert editors will edit your manuscript for grammar, spelling, and other language errors so your ideas are presented at their best.

Preparing Graphics

The quality of illustrations in ACS journals and partner journals depends on the quality of the original files provided by the authors. Figures are not modified or enhanced by journal production staff. All graphics must be prepared and submitted in digital format.

Graphics should be inserted into the main body whenever possible. Please see Appendix 2 for additional information.

Any graphic (figure chart, scheme, or equation) that has appeared in an earlier publication should include a [credit line](#) citing the original source. Authors are responsible for [obtaining written permission](#) to re-use this material.

Figure and Illustration Services

The impact of your research is not limited to what you can express with words. Tables and figures such as graphs, photographs, illustrations, diagrams, and other visuals can play a significant role in effectively communicating your findings. Our [Artwork Editing](#) and [Graphical Abstract](#) services generate publication-ready figures and Table of Contents (TOC) graphics that conform to your chosen journal's specifications. For figures, this includes changes to file type, resolution, color space, font, scale, line weights, and layout (to improve readability and professional appearance). For TOC graphics, our illustrators can work with a rough sketch or concept or help extract the key findings of your manuscript directly for use as a visual summary of your paper.

Preparing for Submission

Manuscripts, graphics, supporting information, and required forms, as well as manuscript revisions, must all be submitted in digital format through [ACS Paragon Plus](#), which requires an ACS ID to log in. Registering for an ACS ID is fast, free, and does not require an ACS membership. Please refer to Appendix 1 for additional information on preparing your submission

Prior Publication Policy

The Journal of Organic Chemistry considers for publication only original work that has not been previously published and is not under consideration for publication elsewhere. When submitting a manuscript, the authors should inform the editor of any prior dissemination of any portion of the

content in print or electronic format, whether available openly to the public or under restricted access. This includes electronic posting of conference presentations (with the exception of short abstracts), posters, and preprints on institutional repositories and on personal Web sites. The exception to these restrictions is the [final version of a thesis](#) filed as a publicly stated requirement for an undergraduate, masters, or Ph.D. degree posted on the official Web site of the degree-granting institution. Authors are allowed to deposit an initial version of their manuscript in a preprint repository such as [ChemRxiv](#), arXiv, bioRxiv, or the applicable repository for their discipline prior to submission. Authors must note any use of a preprint repository in the cover letter, include a link to the preprint, and as appropriate state how the manuscript has been adjusted/updated between preprint deposition and journal submission. The preprint should be cited as a reference in the manuscript. Authors are discouraged from posting a preprint or a revised version of the manuscript as a preprint after the manuscript has been submitted to the journal without consulting with the Editor-in-Chief.

Editorial Policies

Article Based on a Preliminary Report. If the manuscript is an elaboration of a published or “in press” letter or communication, the preliminary report must be mentioned in the cover letter and cited in the introductory remarks in the manuscript (see the policy on prior publication). A copy of the report *and any associated supporting information* must be uploaded as supporting information for review only.

Previous Submission. If substantially the same manuscript has been previously submitted to this or another ACS journal, the cover letter must mention the earlier submission with manuscript number and handling editor name and provide a rationale for reconsideration. If the manuscript was reviewed, copies of all of the reviews should be appended to the cover letter file or uploaded as “Other files for Editors only,” and the cover letter should include a detailed explanation of any revisions, whether or not they were made in response to reviewer and editor comments; an annotated copy of the prior manuscript showing these revisions is welcome.

Permission for Use of Work of Others. A copy of a letter or e-mail message of permission is required when an author cites a personal communication or unpublished results from a researcher who is not a coauthor. This requirement does not apply to data from commercial or in-house service laboratories.

A manuscript incorporating text, tables, or graphics from a copyrighted publication must be accompanied by a copy of a letter or message from the copyright holder identifying the material and granting permission to reproduce it. Permission is not needed when the material is from a paper by one or more of the coauthors published in an ACS journal.

The permission letter or message should be appended to the cover letter file or uploaded as “Other files for Editors only.” If the letter or message is not available at the time the manuscript is submitted, it should be sent to the editor as soon as it becomes available.

Information for Reviewers. *The Journal of Organic Chemistry* operates under a single-anonymized peer review process. The quality of the articles published in the peer-reviewed chemical literature depends heavily on the thoroughness and rigor of the manuscript evaluations provided by reviewers. In addition, the editors of *The Journal of Organic Chemistry* rely on each reviewer’s conscientiously prepared comments for helping maintain the high scientific standards of the journal. Please read the general information about [ACS Peer Review](#) and [ACS Publication Policies](#).

To help facilitate timeliness in the peer-review process, reviewers are expected to promptly respond to invitations to conduct a review and to promptly return their review before the deadline. The editors ask all reviewers to access the manuscripts they are reviewing and submit their reviews on the ACS Paragon Plus website; manuscript files will not be e-mailed or made available to reviewers by other means.

During their evaluation, reviewers are requested to adhere to the precepts in the “Ethical Obligations of Reviewers of Manuscripts” section of the [ACS Ethical Guidelines for Publication of Chemical Research](#). These include treating the manuscript as a privileged document and disclosing any potential conflict of interest to the editor. The editors will not disclose the names of any reviewer to the author of a manuscript. Reviewers should keep the reviewing process confidential by not contacting authors about the content of manuscripts, or disclosing to authors their role as reviewer, without prior approval of the editor. If a manuscript declined by JOC is later submitted to a different ACS journal, the names of the reviewers and copies of the reviews will be made available if requested by the editor of that journal.

Reviewers should become familiar with this complete Author Guidelines document; tools for viewing Supporting Information are [provided here](#). Comments about the content of the manuscript should be entered in the “Comments to the Author” section of the review form. These comments are seen by the editor as well as by the author. Review comments should be objective, impersonal, and constructive. The “Comments to the Editorial Office” section of the form should be used only for ethical concerns and other remarks intended for the editor only.

For the invited reviewer, you might on occasion ask a postdoctoral researcher or graduate student in your group to review the manuscript along with you. This approach is acceptable so long as the reviewer enters a note in the “Comments to the Editorial Office” section of the form when the review is returned. We encourage junior group members to first complete the [ACS Reviewer Lab](#).

Reviewing manuscripts is recognized as a professional obligation of scientists who themselves publish in the literature. Editors are aware of the demands placed on reviewers and have individual reviewer records available to help avoid assigning multiple reviews simultaneously or for making review requests too often.

Reviewer Credit. Reviewers of manuscripts submitted to ACS journals may claim credit for their hard work and contributions through an ACS collaboration with ORCID. Reviewers will receive one credit on their ORCID account for all review activity associated with each manuscript. To claim credit, simply ensure that your ORCID iD is associated with your ACS Paragon Plus account. If you do not have an ORCID iD, you can create one using the ORCID link on your ACS Paragon Plus profile page. For more information, [click here](#).

Note for Authors about Reviews. As an ethical obligation, authors are expected to clearly and succinctly address *all* reviewer comments and concerns during manuscript revision and note how the manuscript has been revised, with an eye toward improving their manuscript. Authors are encouraged to include “for review only” a tracked changes manuscript for revisions and for resubmissions.

Appeals. Appealing an editorial rejection decision is always an option available to authors, one that the Editorial Team takes seriously. But such appeals must be based on rational arguments focused specifically on why a decision should be overturned. Appeals may be successful if they address objective issues (such as interpretation of data, for example) with calm and clear arguments rather than emotional pleas, and address all of the critiques rather than focusing

selectively on positive parts of the reviews and ignoring negative comments. Appeals are less likely to be successful if the rejection of the manuscript was based on the Editor's view that the work does not accommodate the broad readership of the journal (scope). During an appeal, the Editors may obtain additional opinions from other Editors or members of the Editorial Advisory Board before coming to a decision. Authors should not resubmit a rejected manuscript without approval from the journal editorial office.

Previous Submission. If substantially the same manuscript has been previously submitted to this or another ACS journal, the cover letter must mention the earlier submission with manuscript number and handling editor name and provide a rationale for reconsideration. If the manuscript was reviewed, copies of all of the reviews should be appended to the cover letter file or uploaded as "Other files for Editors only," and the cover letter should include a detailed explanation of any revisions, whether or not they were made in response to reviewer and editor comments; an annotated copy of the prior manuscript showing these revisions is welcome.

Providing Potential Reviewer Names

To help the editors identify reviewers with appropriate expertise, please suggest at least three reviewers, avoiding those who coauthored recent publications with any of the authors or who have a close academic or private relationship. ACS requests that you consider the gender and geographic diversity of your suggested reviewers in addition to their topical expertise. Authors are encouraged to give reasons for their suggestions. You may also ask editors to exclude certain reviewers and you may suggest a handling editor. Authors are encouraged to avoid suggesting reviewers from the authors' institutions. Do not suggest reviewers who may have a [real or perceived conflict of interest](#). Whenever possible, suggest academic email addresses rather than personal email addresses.

Manuscript Transfer

If your submission is declined for publication by this journal, the editors might deem your work to be better suited for another ACS Publications journal or partner journal and suggest that the authors consider transferring the submission. [Manuscript Transfer](#) simplifies and shortens the process of submitting to another ACS journal or partner journal, as all the coauthors, suggested reviewers, manuscript files, and responses to submission questions are copied to the new draft submission. Authors are free to accept or decline the transfer offer.

Note that each journal is editorially independent. 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.

PRODUCTION AND PUBLICATION

Proofs via ACS Direct Correct

Correction of the galley proofs is the responsibility of the Corresponding Author. The Corresponding Author of an accepted manuscript will receive e-mail notification and complete instructions when page proofs are available for review via [ACS Direct Correct](#). Extensive or important changes on page proofs, including changes to the title or list of authors, are subject to review by the editor.

It is the responsibility of the Corresponding Author to ensure that all authors listed on the manuscript agree with the changes made on the proofs. Galley proofs should be returned within 48 hours in order to ensure timely publication of the manuscript.

Publication Date and Patent Dates

Accepted manuscripts will be published on the ACS Publications Web site as soon as page proofs are corrected and all author concerns are resolved. The first date on which the document is published on the Web is considered the publication date.

Publication of manuscripts on the Web may occur weeks in advance of the cover date of the issue of publication. Authors should take this into account when planning their patent and intellectual property activities related to a document and should ensure that all patent information is available at the time of first publication, whether ASAP or issue publication.

All articles published ahead of print receive a unique Digital Object Identifier (DOI) number, which is used to cite the manuscript before and after the paper appears in an issue. Additionally, any supplemental information submitted along with the manuscript will automatically be assigned a DOI and hosted on Figshare to promote open data discoverability and use of your research outputs.

ASAP Publication

Manuscripts will be published on the “ASAP Articles” page on the web as soon as page proofs are corrected and all author concerns are resolved. ASAP publication usually occurs within a few working days of receipt of page proof corrections, which can be several weeks in advance of the cover date of the issue.

Post-Publication Policies

The American Chemical Society follows guidance from the [Committee on Publication Ethics](#) (COPE) when considering any ethical concerns regarding a published article, Retractions, and Expressions of Concern.

Additions and Corrections

Additions and Corrections may be requested by the author(s) or initiated by the Editor to address important issues or correct errors and omissions of consequence that arise after publication of an article. All Additions and Corrections are subject to approval by the Editor, and should bring new and directly relevant information and corrections that fix scientific facts. Minor corrections and additions will not be published. Readers who detect errors of consequence in the work of others should contact the corresponding author of that work.

Additions and Corrections must be submitted as new manuscripts via the ACS Publishing Center by the Corresponding Author for publication in the “Addition/Correction” section of the Journal. The corresponding author should obtain approval from all coauthors prior to submitting or provide evidence that such approval has been solicited. The manuscript should include the original article title and author list, citation including DOI, and details of the correction.

Retractions

Articles may be retracted for scientific or ethical reasons and may be requested by the article author(s) or by the journal Editor(s), but are ultimately published at the discretion of the Editor. Articles that contain seriously flawed or erroneous data such that their findings and conclusions cannot be relied upon may be retracted in order to correct the scientific record. When an article is retracted, a notice of Retraction will be published containing information about the reason for the Retraction. The originally published article will remain online except in extraordinary circumstances (e.g. where deemed legally necessary, or if the availability of the published content poses public health risks).

Expressions of Concern

Expressions of Concern may be issued at the discretion of the Editor if:

- there is inconclusive evidence of research or publication misconduct by the authors;
- there is evidence that the findings are unreliable but the authors' institution will not investigate the case;
- an investigation into alleged misconduct related to the publication either has not been, or would not be, fair and impartial or conclusive;
- an investigation is underway but a judgment will not be available for a considerable time.

Upon completion of any related investigation, and when a final determination is made about the outcome of the article, the Expression of Concern may be replaced with a Retraction notice or Correction.

Sharing Your Published Article

At ACS Publications, we know it is important for you to be able to share your peer reviewed, published work with colleagues in the global community of scientists. As sharing on sites known as scholarly collaboration networks (SCNs) is becoming increasingly prevalent in today's scholarly research ecosystem, we would like to remind you of the many ways in which you, a valued ACS author, can [share your published work](#).

Publishing open access makes it easy to share your work with friends, colleagues, and family members. In addition, ACS Publications makes it easy to share your newly published research with ACS Articles on Request (see below). Don't forget to promote your research and related data on social media, at conferences, and through scholarly communication networks. Increase the impact of your research using the following resources: [Altmetrics](#), [Figshare](#), [ACS Certified Deposit](#)

E-Prints

When your article is published in an ACS journal or partner journal, corresponding authors are provided with a link that offers up to 50 free digital prints of the final published work. This link is valid for the first 12 months following online publication, and can be shared via email or an author's website. After one year, the access restrictions to your article will be lifted, and you can share the [Articles on Request](#) URL on social media and other channels. To access all your Articles on Request links, log in to your ACS Researcher Resources account and visit the "My Published Manuscripts" page.

Reprints

[Article](#), [journal](#), and [commercial](#) reprints are available to order.

Appendix 1: PREPARING FOR SUBMISSION

We've developed ACS' publishing and editorial policies in consultation with the research communities that we serve, including authors and librarians. Browse our policies below to learn more.

Ethical Guidelines

ACS editors have provided [Ethical Guidelines](#) for persons engaged in the publication of chemical research—specifically, for editors, authors, and reviewers. Each journal also has a specific [policy on prior publication](#).

OFAC Compliance

As a U.S.-based non-profit organization, the American Chemical Society (ACS) is required to comply with U.S. sanctions laws and regulations administered by the [U.S. Treasury Department's Office of Foreign Assets Control](#) (OFAC). While these laws and regulations permit U.S.-based publishers like ACS to engage in publishing-related activities with authors located in sanctioned regions in many cases, ACS may be prohibited under U.S. law from engaging in publishing-related activities in some cases, including, but not limited to, instances where an author or the institution with which an author is affiliated is located in a particular sanctioned region or has been designated by OFAC as a [Specially Designated National](#) (SDN) pursuant to certain U.S. sanctions programs. ACS reserves the right to refrain from engaging in any publishing-related activities that ACS determines in its sole discretion may be in violation of U.S. law.

Safety Considerations

Authors must emphasize any unexpected, new, and/or significant hazards or risks associated with the reported work. This information should be in the Experimental Section of a full article and included in the main text of a letter. Statement examples can be found in the [Safety Statement Style Sheet](#) and additional information on communicating safety information from the *ACS Guide to Scholarly Communication* [is freely available here](#).

Conflict of Interest Disclosure

A statement describing any financial conflicts of interest or lack thereof is published in each ACS journal and partner journal article.

During the submission process, the Corresponding Author must provide a statement on behalf of all authors of the manuscript, describing all potential sources of bias, including affiliations, funding sources, and financial or management relationships, that may constitute conflicts of interest. If the manuscript is accepted, the statement will be published in the final article.

If the manuscript is accepted and no conflict of interest has been declared, the following statement will be published in the final article: "The authors declare no competing financial interest."

Plagiarism

In publishing only original research, ACS is committed to deterring plagiarism, including self-plagiarism. ACS Publications uses CrossCheck's iThenticate software to screen submitted manuscripts for similarity to published material. Note that your manuscript may be screened during the submission process.

Further information about plagiarism can be found in Part B of the [Ethical Guidelines to Publication of Chemical Research](#). See also the [press release](#) regarding ACS' participation in the CrossCheck initiative.

Authorship, Author List, and Coauthor Notification

Authors are required to obtain the consent of all their coauthors prior to submitting a manuscript. The submitting author accepts the responsibility of notifying all coauthors that the manuscript is being submitted.

During manuscript submission, the submitting author must provide contact information (full name, email address, institutional affiliation, and mailing address) for all of the coauthors. Because all of the author names are automatically imported into the electronic [Journal Publishing Agreement](#), the names must be entered into the submission system. (Note that coauthors are not required to register in the ACS Publishing Center.) Author affiliation should reflect where the work was completed, even if the author has since left that institution. Authors may include a note with a current address if their institution has changed since the work was completed.

To expedite the processing of your manuscript, please format your author and affiliation information according to the guidelines in this [document](#).

Criteria for authorship can be found in Part B of the [Ethical Guidelines to Publication of Chemical Research](#). Artificial intelligence (AI) tools do not qualify for authorship. The use of AI tools for text or image generation should be disclosed in the manuscript within the Acknowledgment section with a description of when and how the tools were used. For more substantial use cases or descriptions of AI tool use, authors should provide full details within the Methods or other appropriate section of the manuscript.

If any change in authorship is necessary after a manuscript has been submitted, confirmation is required that all of the authors (including those being added or removed) have been notified and have agreed to the change. To provide this confirmation, authors are asked to complete and sign an [authorship change form](#) and provide the completed form to the appropriate editorial office.

Authors with a single name: If you, or any of your coauthors, have only one name, please follow these steps for proper submission to the ACS Publishing Center:

1. First (Given) Name Field: Enter an asterisk (*) into the "First (Given) Name" field.
2. Last (Family) Name Field: Enter your single name into the "Last (Family) Name" field.

If your paper is accepted, the asterisk (*) will be removed from the published version of the paper.

Patent Activities and Intellectual Property

Authors are responsible for ensuring that all patent activities and intellectual property issues are satisfactorily resolved prior to first publication (ASAP or in issue). Acceptance and publication will not be delayed for pending or unresolved issues of this nature.

Open Researcher and Contributor ID (ORCID)

Authors submitting manuscript revisions are required to provide their own personal, validated ORCID iD before completing the submission, if an ORCID iD is not already associated with their ACS Publishing Center user profiles. This ID may be provided during original manuscript submission or when submitting the manuscript revision. All authors are strongly encouraged to register for an ORCID iD, a unique researcher identifier. The ORCID iD will be displayed in the published article for any author on a manuscript who has a validated ORCID iD associated with ACS when the manuscript is accepted.

ORCID iDs should not be typed into the manuscript. ACS publishes only those ORCID iDs that have been properly verified and linked **before the manuscript is accepted**. After your ORCID iD is linked, it will be displayed automatically in all subsequently accepted manuscripts for any/all ACS journals. We do not publish ORCID iDs provided during proof review or via other communications after a manuscript is accepted for publication.

With an ORCID iD, 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. If you do not yet have an ORCID iD, or you wish to associate your existing ORCID iD with your ACS Publishing Center account, you may do so by clicking on “Profile” from your ACS Publishing Center dashboard and following the ORCID-related links. Learn more at www.orcid.org.

Copyright and Permissions

To obtain forms and guidelines for completing the Journal Publishing Agreement or obtaining permissions from copyright owners, and to explore a Copyright Learning Module for chemists, click [here](#).

Funder Reporting Requirement

Authors are [required to report funding sources](#) and grant/award numbers. Enter **ALL** sources of funding for **ALL** authors in **BOTH** the Funder Registry Tool in the submission system and in your manuscript to meet this requirement.

Open Access Compliance

ACS offers options by which authors can fulfill the requirements for open access and deposition into repositories for funded research. Visit our ACS Open Science site to see [how to fulfill requirements for specific funders](#) and to find out if you are eligible to publish under a [Read + Publish agreement](#) between ACS and your institution. You can also find out more about [Open Access Compliance](#) and [ACS Open Science initiatives](#).

Diversity and Inclusion Statement

During manuscript submission, ACS journal authors have the option to submit a statement sharing information related to diversity and inclusion that is relevant for their paper. If supplying a diversity

and inclusion statement, the corresponding author must provide this on behalf of all authors of the manuscript during the submission process. These statements include but are not limited to analysis of citation diversity and acknowledgment of indigenous land on which research was conducted. Statements expressing political beliefs are not permitted and may be removed by the journal office. All statements are subject to final review by the Editor.

- **Citation Diversity Statement:** The citation diversity statement should appear in the Acknowledgements section of the manuscript. ACS recommends including the following: (1) the importance of citation diversity, (2) the proportion of citations by gender and race/ethnicity for the first and last authors, (3) the method used to determine those proportions and its limitations, and (4) steps taken to by the authors to improve citation diversity in the article. We recognize that one limitation of the current methods is that it cannot account for intersex, non-binary, and transgender people, or Indigenous and mixed-race authors. (Adapted from [BMES/Springer Guidelines](#))
- **Land acknowledgment:** The land acknowledgment statement should appear in the Acknowledgements section of the manuscript. The statement should link to the institutions' formal land acknowledgments on which the research took place, if possible. Further guidance for creating these statements can be found here: <https://nativegov.org/news/a-guide-to-indigenous-land-acknowledgment/>.

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

Cover art should be visually captivating as well as scientifically interesting. No text can be included on the cover, as it should reflect the science using the graphical elements. The cover should not have pictures of persons alive or dead or places/names that are connected to the place where the research was done. Authors should use "About the Cover" description to describe the cover concept and how it relates to the article, and also as a place to acknowledge those who created or contributed toward the cover artwork. If your art is selected for front cover, ACS will send you information about how to request one complimentary 18" by 24" printed poster featuring your work.

The Journal of Organic Chemistry also offers authors a great way to promote their work through [Supplementary Covers](#). Submit your cover idea, artwork, and caption when submitting your manuscript revision in ACS Paragon Plus. If your article is accepted for publication, your suggestion may be selected for use on one of the journal's supplementary covers.

Web Enhanced Objects (WEO)

The Web editions of ACS journals allow readers to view multimedia attachments such as animations and movies that complement understanding of the research being reported.

WEOs should be uploaded in the submission system with 'Web Enhanced Object' selected as the file designation. Consult the list of [compatible WEO formats](#).