Last updated: December 29, 2023 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.

***JOC*Synopses** 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. *JOC*Synopses 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 Publishing Center

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 the ACS Publishing Center for additional information on everything that is needed to prepare (and review) manuscripts for ACS journals and partner journals, such as

- Mastering the Art of Scientific Publication, which shares editor tips about a variety of topics including making your paper scientifically effective, preparing excellent graphics, and writing cover letters.
- Resources on how to prepare and submit a manuscript to ACS Paragon Plus, ACS Publications' manuscript submission and peer review environment, including details on selecting the applicable 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 ACS Paragon Plus. 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 CH_3 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 *JOC*Synopsis 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 *JOC*Synopsis 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 *JOC*Synopsis 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 *JOC*Synopsis.

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)
- ^{1}H 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 *JOC*Synopsis. 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 *JOC*Synopses. 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: ^{1}H NMR spectra for all compounds (PDF)” or “Additional experimental details, materials, and methods, including photographs of experimental setup (DOC)”.

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

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 $^{13}C\{^{1}H\}$ 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, CH_2, CH_3) 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 ^{1}H and ^{13}C NMR data to conform to *the ACS Guide to Scholarly Communication* format is (high to low): ^{1}H NMR (C_6D_6, 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). ^{13}C{^{1}H} NMR (C_6D_6, 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 wellresolved 1D proton NMR spectrum and a copy of a protondecoupled 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 ^{13}C and ^{1}H 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 HMRS 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 $C_{13}H_{17}NO_3$: 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 parentderived 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×(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 [] = (100×)/(*l*×*c*) should be reported as unitless numbers as in the following example: $[]_D^{20}$ -25 (*c* 1.9, $CHCl_3$), where the concentration *c* is in g/l00 mL and the path length *l* is in decimeters. The units of the specific rotation, (deg×mL)/(g×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 cm^{1} 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 signaltonoise 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 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).
- *^{1}H and/or ^{13}C 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 R^2, 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.

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Appendix 2: Preparing Graphics

Resolution

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

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

Size

Graphics must fit a one- or two-column format. Single-column graphics can be sized up to 240 points wide (3.33 in.) and double-column graphics must be sized between 300 and 504 points (4.167 in. and 7 in.). The maximum depth for all graphics is 660 points (9.167 in.) including the caption (allow 12 pts. For each line of caption text). Lettering should be no smaller than 4.5 points in the final published format. The text should be legible when the graphic is viewed full-size. Helvetica or Arial fonts work well for lettering. Lines should be no thinner than 0.5 point.

Color

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

Type of Graphics

Table of Contents (TOC)/Abstract Graphic

Consult the Guidelines for Table of Contents/Abstract Graphics for specifications.
Our team of subject-matter experts and graphical designers can also help generate a compelling TOC graphic to convey your key findings. Learn more about our Graphical Abstract service.

Figures

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

Charts

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

Tables

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

Schemes

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

Chemical Structures

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

Cover Art

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.

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