IMPORTANT MANUSCRIPT SUBMISSION REQUIREMENTS

Notes and JOCSynopses are limited to 3000 and 4000 words, respectively; tables and graphics count toward the word-count limits at the rate of 50 words per vertical inch for one-column (<3.3 inches wide) items, and 100 words per vertical inch for wider items. The Note word-count limits does not include the experimental section. For information about the length limit for JOCSynopses see section 2.3.3.

During online submission, the names of all the coauthors must be entered in step 2 in the same sequence and form as they appear on the first page of the manuscript.

All experimental procedures and compound characterization data should appear in the manuscript's experimental section and not the supporting information.

For new compounds, ensure required data are furnished in the experimental section and supporting information, including either MS accurate mass or elemental analysis data, proton and carbon NMR data (combined together in the supporting information file), and any CIF files.

The manuscript and supporting information files should be free of font and graphics-quality problems and should not have extensive English usage or grammar deficiencies.

All tables and graphics (figures, reaction schemes, and chemical structures) are inserted within the manuscript text where they are first discussed (except for TeX/LaTeX submissions).

The references and endnotes must be grouped into a single list at the end of the manuscript file.

A supporting information availability statement that lists the types of data in the supporting information files is included in the manuscript file.

A Compound Characterization Checklist is furnished if the manuscript reports characterization data for new compounds or known compounds prepared by a new or modified method.

Previous submission of the same manuscript to another journal must be disclosed in the cover letter. For reviewed submissions, include in the cover letter a detailed explanation of changes made and copies of the reviews as “Other files for Editors only”.

Upload as “Supporting Information for Review Only” any published preliminary report and associated supplementary material; mention the report in the cover letter and cite in the manuscript’s introductory remarks.

Provide a copy of any cited “in press” or “submitted-for-publication” paper as “Supporting Information for Review Only”.
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1 Scope and Editorial Policy

1.1 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 originality of the work as well as the breadth of interest to the organic chemistry community.

Total synthesis and other multistep synthesis manuscripts are expected to demonstrate novel strategies, new synthetic transformation methods, or shortened routes to target structures. Manuscripts illustrating new synthetic methods need to show conceptual novelty, not merely the extension of previously reported chemistry to a different class of reaction substrates, reagents, or catalysts. Natural products isolation and identification studies should report unusual skeletal features, improvements in identification methods, or insights into biosynthetic pathways. Manuscripts with a major component of biology, analytical chemistry, or materials science should demonstrate novelty in the organic chemistry portion of the work being reported.

1.2 Types of Papers Published

Articles are comprehensive, critical accounts of the solution of significant problems. Articles based on work reported in a preliminary letter or communication are welcome provided that 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 that were reported in the preliminary publication may be included when the author feels 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 (see section 3.2.3).

Featured Articles are Articles that have been selected by the editors for their quality, interest, and importance, and have also received especially strong positive comments from the reviewers. They 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 Web site.

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 3000 words, exclusive of the experimental section and the list of references and endnotes. For Notes, the space occupied by tables and graphics is charged against the word count (see section 2.3.3).

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. They are limited to 4000 words of text and 80 references and endnotes (see section 2.3.3). JOCSynopses are invited or are submitted and screened before a formal review.

Perspectives are personal overviews of specialized research areas by acknowledged experts. They are published only by invitation of the Editor-in-Chief.

1.3 Manuscript Requirements

Manuscripts should be submitted on the American Chemical Society (ACS) Paragon Plus Web site at
A manuscript submitted to *The Journal of Organic Chemistry* must be based on original research by the authors. Web posting of any content in a manuscript (with the exception of short abstracts), whether available openly to the public or under restricted access, must be disclosed to the editor and may compromise the originality of the submitted manuscript. 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.

At the time a manuscript is submitted to *JOC*, and during the time it is under evaluation, no other manuscript reporting the same results may be under simultaneous consideration by another journal. Manuscripts declined by other journals will be considered if their focus is appropriate for publication in *The Journal of Organic Chemistry*. Manuscripts previously considered and declined by *The Journal of Organic Chemistry* may not be resubmitted except when the editor has invited submission of a new manuscript incorporating specified additions or changes. If the editor agrees to reconsider a rejected manuscript that has been rewritten at the editor’s suggestion to accommodate the reviewers’ or editor’s objections, the revision will be treated as a new submission, will be given a new “Received” date, and will be assigned to the same editor.

### 1.4 Manuscript Evaluation

The editors have final authority regarding all decisions concerning submitted manuscripts. Although they generally consider the advice of scientific peers, they may decline without review manuscripts judged inappropriate for the Journal or in violation of the ACS Ethical Guidelines.

The author may express a preference in the cover letter for the manuscript to be assigned to a particular associate editor. The Editor-in-Chief’s selection of an associate editor will take into account the author’s suggestion and the availability, workloads, and areas of expertise of the editors. An editor-invited resubmission of a manuscript that has been previously submitted to this Journal will be handled by the original editor.

During the manuscript submission process, the author is required to enter the names and e-mail addresses of at least five researchers qualified to act as reviewers. An author may request in the cover letter that a certain person not be used as a reviewer. Such a request will be honored unless the editor feels that individual’s opinion, in conjunction with the opinions of other reviewers, is vital for evaluating the manuscript. The names of reviewers will not be revealed to authors.

Reviewers are asked to evaluate manuscripts on significance, scientific rigor, originality, breadth of interest to the organic chemistry community, thoroughness of compound characterization, appropriateness of cited literature, and quality of writing. An editor will consider, but will not always follow, the recommendations of the reviewers.

If the reports of the reviewers are generally positive, the editor may request the author to furnish a revised manuscript that appropriately addresses any reviewer and editor concerns. The editor may send the revised manuscript to the original reviewers or to new reviewers, or may reach a decision based on the original reviews and the author’s response to them, without seeking further opinions.

If substantially the same manuscript has been previously submitted to this or another ACS journal, the author should disclose the journal name and manuscript number in the cover letter. If the manuscript was reviewed, the author should attach copies of all the reviews to the cover letter, and provide a detailed explanation of the changes made in response to the reviewer comments. The editor may request the names of the original reviewers and copies of the reviews from the editor of the other ACS journal. The editor may accept the manuscript on the basis of the original reviews and the author’s changes, seek additional reviews, or reject the manuscript without further review.
1.5 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 and suggest that the authors consider transferring the submission. The Manuscript Transfer Service simplifies and shortens the process of submitting to another ACS journal, as all the coauthors, suggested reviewers, manuscript files, and responses to submission questions are copied by ACS Paragon Plus to the new draft submission. Authors are free to accept or decline the transfer offer.

Once a transfer is accepted, authors will then complete the submission to the new journal in ACS Paragon Plus. During the submission process, they will have the opportunity to revise the manuscript and address comments received from editors or reviewers. Requirements of the new journal may be different, so authors should also check the Author Guidelines for the new journal and make any needed revisions in order to conform to those requirements. Please keep in mind that the reviews, reviewer identities, and decision letter will all be transferred to the new journal. Authors are encouraged to identify changes made to the manuscript in a cover letter for the new journal.

Note that transferring a manuscript is not a guarantee that the manuscript will be accepted, as the final publication decision will belong to the editor in the new journal. For complete details, see http://pubs.acs.org/page/policy/manuscript_transfer/index.html.

1.6 Funding Sources

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

1.6.1 Institution Identification

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

1.7 Ethical Considerations

The Journal expects editors, reviewers, and authors to adhere to the standards embodied in the American Chemical Society's Ethical Guidelines to Publication of Chemical Research. Those guidelines are available on the Paragon Plus Web site at http://pubs.acs.org/page/policy/ethics/index.html.

Manuscripts must be original with respect to concept, content, and writing. It is not appropriate for an author to reuse wording from an earlier publication, whether or not that publication is cited. 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.

Spectra, photographs, and other images may not be altered in a way that misrepresents the experimental results or misleadingly presents them in a more favorable manner. Any editing of an image must be clearly disclosed in a footnote below the image.

Authors are reminded of their obligation to obtain the consent of all their coauthors prior to submitting a manuscript for publication. If any change in authorship is necessary after a manuscript has been submitted, the corresponding author must e-mail or fax a copy of a signed letter to the Editor-in-Chief confirming that all of the original coauthors have been notified and have agreed to the change. If the change involves the removal of a coauthor’s name, the corresponding author must also arrange for the coauthor involved to e-mail or fax a copy of a separate signed letter consenting to the change. No changes in the author list will be permitted after a manuscript has been accepted.
A statement describing any financial conflicts of interest or lack thereof must be included with each manuscript. During the submission process, the corresponding author must provide this statement on behalf of all authors. The statement should describe all potential sources of bias, including affiliations, funding sources, and financial or management relationships, that may constitute conflicts of interest (please see the ACS Ethical Guidelines). The statement will be published in the final article. If no conflict of interest is declared, the following statement will be published in the article: “The authors declare no competing financial interest.”

1.8 Online Publication

The Journal is published biweekly in printed and online editions.

1.8.1 Articles ASAP

The copyedited final versions of accepted papers are published as Articles ASAP (As Soon As Publishable) on the Journal web site, usually within four working days of receipt of the author’s page proof corrections. A Digital Object Identifier (DOI) of the form 10.1021/acs.joc.xxxxxxxx is assigned to each accepted manuscript. Authors are given instructions for citing their work by DOI in an e-mail when the manuscript proofs are made available. The DOI may be used to cite the paper both before and after it appears in a numbered issue of the Journal.

1.8.2 Just Accepted Manuscripts

Just Accepted manuscripts are peer-reviewed, accepted manuscripts that are posted on the ACS Publications Web site prior to technical editing, formatting for publication, and author proofing, usually within 30 minutes to 24 hours of acceptance by the editorial office. During the manuscript submission process, an author can choose to have the manuscript posted online as a Just Accepted manuscript. No supporting information or Web enhanced object files are included with a Just Accepted manuscript. To ensure rapid delivery of the accepted manuscript to the Web, authors must adhere carefully to all requirements in these Guidelines for Authors. If the author accepts this publication option, the official publication date is the date on which the manuscript is posted on the Journal’s ‘Just Accepted Manuscripts’ Web page, rather than the date on which the copyedited and proof-corrected version is published on the Articles ASAP page. Just Accepted manuscripts can be cited by DOI as described above. Authors should take the Just Accepted manuscript publication date (or the Articles ASAP publication date if the Just Accepted manuscript option is not elected) into account when planning patent or other time-sensitive activities. Once a manuscript appears on the Web, it is considered published. After that point, any change must be submitted for publication as an Addition or Correction (see section 3.6). For further information, please refer to the ‘Frequently Asked Questions about Just Accepted Manuscripts’ Web page at http://services.acs.org/pubshelp/passthru.cgi?action=kb&item=244. Note that publication as a Just Accepted manuscript is not a means of complying with the NIH Public Access Mandate.

2 Preparing the Manuscript and Supporting Information

2.1 Manuscript Organization

In general, manuscripts must contain: (1) Title, (2) Authors’ names and addresses, (3) Corresponding author’s e-mail address, (4) Table of Contents/Abstract Graphic, (5) Abstract, (6) Introduction, (7) Results and Discussion [may be separate], (8) Conclusion [optional], (9) Experimental Section [except Perspectives, JOCSynopses, and accounts of purely theoretical studies], (10) Acknowledgments [optional], (11) Supporting Information availability statement [required if the manuscript is accompanied by any supporting information for publication], and (12) References and Endnotes.

Section Headings. The only section headings used in a Note are Experimental Section,
Acknowledgments, and Supporting Information. An Article has, in addition, Introduction, Results and Discussion, and Conclusion (optional) section headings. A JOCSynopsis has the same section headings as a Note except that there is no Experimental Section. Papers published in JOC do not contain sections titled Abbreviations or Appendix.

2.1.1 Title
The title should accurately, clearly, and concisely identify the subject and emphasis of the reported work. Words should be chosen carefully to reflect the content and to function as indexing terms. Abbreviations should be avoided. Manuscript titles should not make claims of priority, originality, convenience, effectiveness, or value. For example, the words “convenient”, “efficient”, “elegant”, “expedient”, “facile”, “first”, ”new”, “novel”, ”practical”, ”simple”, “unique”, “unprecedented”, and ”versatile” should not be used. In addition, editors may ask authors to moderate or remove what they judge to be excessive use of subjective evaluative language elsewhere in manuscripts. Neither the title nor any other text should indicate that the paper is part of a numbered series on a broader research topic, or a numbered contribution from a particular institution or research group.

2.1.2 Authors’ Names and Addresses
The names of the coauthors are listed below the title. A consistent format should be used, preferably given name, middle initial (if any), and surname. The name of the corresponding author(s) should be marked with an asterisk (*). The names and addresses of the institution(s) where the work was performed should be listed immediately below the coauthor names. If the coauthors are not all at the same institution or department, the institutional affiliation of each author should be indicated by labeling the institution names, using the typographic symbols †, ‡, §, and ¶, and placing those symbols as superscripts after the appropriate author names. If a corresponding author is no longer at the institution where the work was performed, a footnote, marked with an asterisk (*) rather than a number, should give that author’s current address.

2.1.3 Corresponding Author’s E-mail Address
The e-mail address of the corresponding author should be placed on a separate line below the institution addresses; if there are two corresponding authors, e-mail addresses for both should be listed. All editorial correspondence concerning receipt, review, revision, and publication of a manuscript will be sent by e-mail to the coauthor designated as the corresponding author during the online manuscript submission process, even if the manuscript is submitted by a different individual.

2.1.4 Table of Contents/Abstract Graphic
The content and formatting of the table of contents graphic are discussed in section 2.5.5.

2.1.5 Abstract
The abstract for an Article or Note should briefly state the purpose of the research, the principal results, and the major conclusions. A well written abstract can attract the attention of potential readers and increase the likelihood that the published paper will get 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").

For a JOCSynopsis or Perspective, the abstract should identify the scope and focus of the manuscript. The length of the abstract for a Note or JOCSynopsis is limited to 80 words. The length of the abstract for an Article should not exceed 200 words. Undefined nonstandard abbreviations and reference citation numbers should be avoided.
2.1.6 Introduction
The introduction should place the work in the appropriate context 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.

2.1.7 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.

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

2.1.9 Experimental Section
For Notes and Articles, every manuscript reporting the results of experimental work must include an experimental section, and all experimental procedures, compound characterization data, and any associated literature citations must appear in the manuscript’s experimental section. This section should describe experimental methods in sufficient detail to permit repetition of the work by others. These procedures and data listings should not be duplicated in the supporting information. Section 2.2 (‘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.

Authors must emphasize any unexpected, new, and/or significant hazards or risks associated with the reported work. This information should be in the experimental details section of the full article or Note.

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 should be placed at the beginning of the experimental section.

Sources of stationary phases for chromatography and supports for solid-phase 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.

2.1.10 Acknowledgments
This section may be used to acknowledge discussions with other researchers, technical assistance, gifts of starting materials or reference samples, data from institutional or individual providers of spectroscopic, analytical, or crystallographic services, and financial support. A funding provider for an instrument may be thanked. Authors whose cover art submissions are used may later add recognition of the graphic artist.

2.1.11 Supporting Information Statement
If the manuscript is accompanied by any supporting information files for publication, a brief description
of each file is required. The paragraph and descriptions should be placed at the end of the manuscript before the list of references. The appropriate format is:

**Supporting Information.** Brief descriptions in nonsentence format listing the contents of the files supplied as Supporting Information.

### 2.1.12 References and Endnotes

All references and any explanatory endnotes must be numbered in a consecutive list at the end of the manuscript text. The references and endnotes should be entered as superscripts in the text and numbered in the order of their first appearance. Authors are asked to assign a separate number to each citation (and to cite them as, for example, 4–9) rather than nest several citations under a single reference number (4, 5, 6). If an endnote needs to refer to a numbered reference elsewhere in the References and Endnotes section, the reference number should not be superscripted (for example, “see reference 14”).

In the published versions of the paper, the references and endnotes will appear together at the end of the text, and references may have links to their abstract and full text on publisher Web sites. Because of this electronic linking, and because the references are not always checked in detail by editors or reviewers, it is crucial that authors verify accuracy.

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 his or her own publications, except in a Perspective or JOCSynopsis. No reference should repeat a reference that appears elsewhere in the manuscript’s list of references. 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. See section 2.3.3 for references and endnote requirements for JOCSynopses.

Authors should consult a recent issue of the Journal or *The ACS Style Guide* (3rd ed., 2006, Oxford University Press, ISBN 0-8412-3999-1) for guidance on the appropriate formats to use in citations of journal papers, books, and other publications. The names of all coauthors of a cited work should be listed in the reference (“et al.” may be used in the text where the work is discussed). Journal title abbreviations should be those used by *Chemical Abstracts* and listed in the *Chemical Abstracts Service Source Index*. The abbreviations for the most frequently cited journal titles may be found in *The ACS Style Guide* or on the Web at [http://www.cas.org/expertise/cascontent/caplus/corejournals.html](http://www.cas.org/expertise/cascontent/caplus/corejournals.html). For patents, for journals not published in English, and for journals that are not easily obtainable by most readers, a *Chemical Abstracts* citation should also be given. DOI numbers should be furnished for new papers awaiting publisher-assigned page numbers (*Articles ASAP* for ACS journals) and for reports published only online. Web pages and documents on maintained institutional repositories may be cited using their URL.

### 2.2 Specialized Data

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

#### 2.2.1 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.
For Notes and Articles, all experimental procedures and listings of compound characterization data must be included in the manuscript experimental section, and not in the supporting information. The supporting information should contain only copies of spectra, chromatograms, graphs, tables, crystallographic data, and computational data.

Fully characterized compounds should have bolded compound names (see section 2.3.5) 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 (section 4) 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. 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 what quantity is being reported. The isolation and purification of the products for several representative 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 to demonstrate the practical utility of the method as a synthetic tool.

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. The Journal 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, manufacturer and model, 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.
2.2.2 Compound Characterization Data

The Journal 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 known yield and purity. For new compounds, evidence adequate to establish both identity and degree of purity (homogeneity) must be provided. Purity documentation must be provided for known compounds whose preparation by a new or modified method is reported. The Journal 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 may be asked to provide copies of original spectra or analytical reports if an editor or reviewer raises a question about any of the reported results.

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 ‘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.

It is generally expected that mixtures of regioisomers, geometric isomers, and diastereomers (but not usually enantiomers) will 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 file’s experimental section. No experimental procedures or listings of compound characterization data, whether for new or known compounds, should appear in the supporting information.

The formatting of spectroscopic, physical, analytical, and other product characterization data should adhere to the recommendations in The ACS Style Guide, 3rd edition, pages 274–276, 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.

A completed Compound Characterization Checklist (see section 3.2.2) must be provided, even if only known compounds were prepared, to help editors and reviewers assess the thoroughness of the identity and purity documentation. New compounds and known compounds that have been prepared by new or modified procedures should be included. Known compounds that have been synthesized by literature methods or obtained from commercial sources should not be listed.

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.

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.** Proton and carbon NMR resonances should be listed for each new compound; the solvent and instrument frequency should be identified. The use of broadband decoupling should be indicated with braces, for example $^{13}$C{[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. 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 (section 2.1.9) 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.

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, unreacted 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.

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.

Refer to the ACS Publishing Tools page for general NMR reporting guidance.

Optionally, authors may furnish a folder of NMR free induction decay (FID) files as additional supporting information. Authors reporting compounds of complex, unusual, or unexpected structure are encouraged to provide FID data. See section 2.6 (‘Supporting Information’) for information about preparing this material for submission. The FID data should be mentioned in the manuscript file’s
Elemental Analysis and Accurate Mass Measurement. For most new compounds except large biomacromolecules (see below) and polymers, 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 ACS Style Guide 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 the first paragraph of section 2.2.2 for the 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 paper 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 Style Guide 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 Style Guide 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 (section 2.2.4) 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.

**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 \([\alpha] = (100 - \alpha)/(\ell - c)\) should be reported as unitless numbers as in the following example: \([\alpha]_D^{20} - 25 (\ell 1.9, \text{CHCl}_3)\), where the concentration \(c\) is in g/100 mL and the path length \(\ell\) is in decimeters. The units of the specific rotation, \((\text{deg} \cdot \text{mL})/\text{g} \cdot \text{dm})\), are implicit and are not included with the reported value.

**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.

**IR and 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, the Journal 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 proton-decoupled 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 vacuum-transferred 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 enzyme-mediated 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.

### 2.2.3 Spectra

Reproductions of spectra will be published in the results and discussion section only when concise numerical summaries are inadequate for the discussion. Papers 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 (see section 2.5.5), should be included. Spectra used as adjuncts to the characterization of compounds should be included in the supporting information.

### 2.2.4 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.

For structures refined anisotropically, a thermal ellipsoid plot, preferably full-page size, should be furnished as a figure in the supporting information; the ellipsoid contour percent probability level should be reported in the caption. A brief text description of the sample preparation and crystal structure determination, 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, since those data are included in the required Crystallographic Information Framework (CIF) file (see below). Spherical-atom or wire-frame models, packing diagrams, stereo views, and other graphics may also be included in the supporting information when appropriate. 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.

A Crystallographic Information Framework (CIF) file containing complete crystallographic data must be furnished as Supporting Information for Publication any time a structure is reported. Reflection intensity data (structure factor tables) are not required. If more than one crystal structure is being reported, the individual CIF files can be submitted as single files or combined and uploaded as a single supporting information file.

CIF files should be saved in text-only (plain ASCII) format and should be assigned file names that identify the structure number used in the manuscript and that include a “.cif” (not “.txt”) extension, for example, Compounds_14, 16, and 23.cif; they should not be incorporated into other types of supporting information files. If the CIF files were deposited with the Cambridge Crystallographic Data Centre prior to manuscript submission, the CCDC deposition numbers may be included with the text description of the structure determination in the supporting information, but copies of the CIF files still need to be furnished as additional supporting information files.

Before being submitted, CIF files should be checked using the free checkCIF data-validation utility on the Paragon Plus Web site at [http://pubs.acs.org/page/4authors/tools/validate_cifs.html](http://pubs.acs.org/page/4authors/tools/validate_cifs.html). Any reported syntax
errors and A, B level alerts should be corrected. Copies of the checkCIF data-validation reports are not required and will not be published. Authors who wish to furnish the checkCIF reports (in addition to the required CIF files) may upload them as Supporting Information for Review Only.

2.2.5 Computational Data

Complete details of computational methods and results should be reported in sufficient detail to allow other researchers to repeat the computations. Relevant input parameters such as specific programs and detailed description of the methods used should be included. Z-matrices or Cartesian coordinates, the number of imaginary frequencies, and computed total energies of target or optimized structures, along with any other absolute energy values used to calculate relative energies reported in the paper, should be placed in the supporting information. This documentation is required even when the theoretical discussion is ancillary to a primarily experimental study. In cases where files larger than 10 MB would be required to report the results, an input file and associated information that would allow reproduction of the calculation is acceptable as documentation. These data should be included on the Compound Characterization Checklist (see section 3.2.2). Graphics that are not integral to the discussion should be placed in the supporting information.

2.2.6 Bioassay Data

Because the scope of this Journal does not include development of new bioassay methods, it is expected that reported bioassay data was 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.

2.3 Manuscript Text

2.3.1 Writing Style and Language Usage

Clarity and conciseness are critical requirements for reports published in the Journal. Authors should consult The ACS Style Guide for guidance on style, chemistry-related word-usage conventions, nomenclature, physical quantity symbols and units, grammar, capitalization, punctuation, and formatting of references. Spelling and use of periods and commas in numbers should conform to U.S. usage. Authors seeking professional assistance with improving the English, figures, or formatting in their manuscript before submission can find resources at ACS ChemWorx Authoring Services. Manuscripts with extensive English usage or grammar deficiencies will not be forwarded to reviewers.

2.3.2 Word-Processor and PDF Versions

Authors who use a word processor (Microsoft Word or Corel WordPerfect) may either submit both a word-processor and a PDF version, or they may submit only the word-processor version and allow Paragon Plus to create the PDF version for their inspection prior to the final step of manuscript submission. Submission of both versions is strongly encouraged to ensure the quality of the graphics in the PDF version seen by the reviewers. Additional information about author-supplied manuscript PDF
files is available here. Because the two versions need to be identical, authors who furnish the PDF version should not further edit the word-processor or TeX/LaTeX version after the PDF version has been created.

2.3.3 Word-Count and Reference-Count Limits

The length of a Note is limited to 3000 words (including text and numerical entries in tables) for the abstract, introductory paragraph, and the results and discussion. Graphics and any tables containing graphics, sized to one-column (3.3 inch) or two-column (7.0 inch) width, are charged against the word-count limits at the rate of 50 words per vertical inch for one-column-wide items, and 100 words per vertical inch for wider items. The experimental section, acknowledgments, supporting information availability statement, and list of references and endnotes are excluded from the word-count limit.

The length of an invited JOCSynopsis is limited to 4000 words, exclusive of the acknowledgments and the list of references and endnotes. All the graphics (and any tables containing graphics) must be able to fit on two U.S. letter-size word-processor pages. More detailed instructions will be furnished to authors at the time the invitation is sent.

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.

The number of references and explanatory endnotes is limited to 80 for a JOCSynopsis. Although no numerical limit is set for Articles and Notes, excessive literature citation, including self-citation, is strongly discouraged (see guidance in section 2.1.12).

2.3.4 Text File Formatting

**Word-Processing Software.** Manuscripts may be prepared with Microsoft Word, Corel WordPerfect, or TeX/LaTeX; a list of versions compatible with the Paragon Plus manuscript submission system can be found here. TeX/LaTeX users should follow the guidelines provided below.

**Using TeX/LaTeX.** Authors who submit manuscripts composed in TeX/LaTeX should submit a PDF file of the manuscript along with the native TeX/LaTeX manuscript package as a ZIP Archive. The submission must include all referenced files, including all necessary resource files such as bibliographic and style files and images. Use of the freely available achemso style package to help prepare the submission is strongly encouraged. The achemso package provides the official macros (achemso.cls) and BibTeX styles (achemso.bst and biochem.bst) for submission to ACS journals. The package and instructions are available from CTAN, the Comprehensive TeX Archive Network. See Preparing and Submitting Manuscripts Using TeX/LaTeX for complete instructions.

**ACS Math Style.** Authors including math, display or in-text, in their manuscripts are encouraged to consult the ACS Guidelines for Presenting Mathematical Information. This style sheet provides brief discussion of formatting related to the presentation of mathematical formulas, complete with examples of ACS style and layout. This document was developed to help authors anticipate how mathematical expressions will be formatted in the published version of the paper.

**Fonts and Typography.** Times, Times New Roman, Helvetica, Arial, or Courier fonts should be used for the text of the manuscript and supporting information files to minimize font-embedding problems when the word-processor file is converted to the PDF and HTML versions seen by the reviewers. The Symbol font must be used for Greek letters and mathematical symbols. The single-character symbol for degrees Celsius found in some fonts may not convert correctly to PDF and should not be used; instead, the degree sign in Symbol font should be followed by the capital letter “C” in the normal text font. The letters O, l, and x should not be substituted for the numerals 0 and 1 and the multiplication symbol ×. Minus signs or ‘en’ dashes, rather than hyphens, should be used for negative quantities.

**Page and Line Numbering.** Paragon Plus automatically adds page numbers and line numbers to the PDF version of the manuscript seen by the reviewers, regardless of whether the author submits the manuscript PDF file or allows Paragon Plus to create it from the word-processor file. Therefore, authors should not include page and line numbers in the submitted manuscript word-processor file or in the optional
Formatting and Page-Size Setting. This Journal does not require the use of a manuscript template and does not provide journal-specific templates.

Placement of Tables and Graphics. All tables and graphics must be inserted into the manuscript near their first mention in the text; they should not be grouped at the end of the text. Unless the manuscript is being submitted as a TeX/LaTeX file, tables and graphics should not be uploaded as individual files.

Saving the File. For new manuscripts, editor-invited resubmissions, and post-review revisions, the word-processor file uploaded as the Manuscript File (and the Manuscript PDF file, if one is furnished) must not be password-protected and must not contain comments, colored text, or color-highlighted text. If the word processor’s Track Changes tool has been used, all changes must be accepted (incorporated as final) before the file is saved and uploaded to Paragon Plus.

2.3.5 Nomenclature
Authors should furnish a correct systematic name, following International Union of Pure and Applied Chemistry (IUPAC) conventions, for each compound whose preparation is reported in the experimental section. Complex compounds with lengthy or unwieldy names may be referred to by their functional class and structure number (for example, ketone 23) elsewhere in the text. Names generated by ChemDraw or other software from inputted graphic formulas should be checked for extra hyphens and other deviations from IUPAC conventions. IUPAC guides to organic and biochemical nomenclature are available on the Web at http://www.acdlabs.com/iupac/nomenclature. For certain specialized classes of compounds such as steroids, peptides, carbohydrates, and cyclophanes, the names should conform to the nomenclature conventions generally accepted for those classes. Systematic or generic names should be used for commercial products rather than proprietary or trademarked names.

The use of italics, capitals, small capitals, hyphens, parentheses, and square brackets for positional, configurational, and stereochemical prefixes and descriptors should conform to the conventions in The ACS Style Guide, 3rd edition, chapter 12 (Names and Numbers for Chemical Compounds). The name and structure number of an enantioenriched compound of known absolute configuration should include a (R) or (S) stereochemical descriptor for each stereogenic center. The (R*,S*) convention should be used where the relative but not the absolute configurations of multiple stereogenic centers in diastereomers are known.

2.3.6 Abbreviations, Physical Quantity Symbols, and Units
Authors are encouraged to use abbreviations and acronyms in the manuscript text. The Journal’s list of standard abbreviations and acronyms is included in section 4. Abbreviations and acronyms not on this list must be defined the first time they are used in the text, and should not be used in the title, abstract, or table of contents/abstract graphic. Papers published in JOC do not include an Abbreviations section in either the manuscript or supporting information files. Authors need to keep in mind that JOC is read by a wide audience of organic chemists, and abbreviations accepted as standard within a specialized area of organic chemistry may not be recognized by readers outside that specialty. The use of abbreviations should be consistent throughout the manuscript text, tables, and graphics. For example, either CH₃ or Me may be used for “methyl”, but not both.

Symbols for physical quantities should be italicized (for example, c, Eₐ, J, m/z, t₁/₂). The International System of Units (SI units) should generally be used, but authors may also use common non-SI metric units such as Å, cal, cm⁻¹, eV, g, Hz, L, ppm, and °C. Abbreviations for units are not italicized, and most are used without a final period.

2.4 Tables
Tables must be inserted in the manuscript word-processor file near their first mention in the text. Tables
should be created with the word processor’s table-formatting feature. Each data entry should be placed within its own table cell; tabs and line returns should not be used within cells. Whenever possible, structure numbers should be used in tables rather than small chemical structure graphics. If a table-formatting feature is not available, adjacent columns should be separated with tabs rather than spaces, and a line return should be inserted at the end of each row. Arrangements that leave many columns only partially filled should be avoided. During production of the PDF version of the paper, tables are generally placed at the top of a column or page. In the HTML version they are inserted after the paragraph in which they are first mentioned.

For Notes, tables count against the word-count limits (see section 2.3.3) at the rate of 50 words per vertical inch for tables up to 3.3 inches wide (single-column width), and 100 words per vertical inch for tables wider than 3.3 inches.

Above each table should be typed, in boldface characters, a sequential Arabic table number and a short descriptive title (for example, TABLE 3. Strain Energies of Substituted Spiropentanones). The title, together with the individual column and row headings and footnotes, should make the table self-explanatory; titles and footnotes containing “see text” should be avoided. If the word processor’s table tool is used, the table number, title, and any footnotes should not be placed in table cells but should be typed above or below the table. No collected list of all the table titles should be included at the end of the manuscript. Each table must be referred to by its number at least once in the manuscript text.

Footnotes for tables should be given lowercase italic letter designations and should be cited in the table with lowercase italic superscripted letters. The sequence of letters should proceed by row and from left to right within any rows having more than one footnote. If a reference needs to be cited in a table, a lettered footnote below the table should include the number assigned to that reference in the list of references at the end of the manuscript.

2.5 Graphics

2.5.1 General Requirements

All graphics must be prepared in digital format [TIFF, PDF, EPS (vector artwork), or CDX (ChemDraw file)], and inserted into the manuscript word-processor file near their first mention in the text. During production of the PDF version of the paper, figures are placed at the top of a column or page. Duplicate copies of manuscript graphics should not be furnished in supporting information or web enhanced object files. Additional guidance on creating graphics for manuscripts may be found in The ACS Style Guide, 3rd edition, chapters 15 (Figures) and 17 (Chemical Structures).

Graphics count against the word-count limits of Notes (see section 2.3.3) at the rate of 50 words per vertical inch for graphics up to 3.3 inches wide (single-column width), and 100 words per vertical inch for graphics wider than 3.3 inches.

No graphics should be included in the experimental section other than individual graphic structures of synthesized products that optionally accompany listings of compound characterization data.

Any graphic (figure, chart, or scheme) that has appeared in an earlier publication should include a footnote directly below the graphic citing the original source. Permission needs to be arranged and documented when a graphic from a copyrighted source other than one of the coauthors’ papers in an ACS journal is reproduced in a manuscript (see section 3.2.1).

Number Figures consecutively with boldface Arabic numerals and brief descriptive captions. The figure number and caption should be typed in the manuscript word-processor file directly below the graphic (rather than included in the graphic). The caption should identify the content of the figure and should be understandable without reference to the text. If a figure has several parts, the individual parts should be labeled (a), (b), etc., and each part identified in the caption. The key to symbols used in a figure (for example, for marking experimental points in a graph) should be included in the figure itself whenever
possible. Each figure must be referred to by its number at least once in the manuscript text. No collected list of the figure captions should be included at the end of the manuscript.

For manuscripts created with TeX/LaTeX, the guidelines on the Paragon Plus Web site at http://pubs.acs.org/page/4authors/submission/tex.html should be consulted.

**Author portrait for Perspectives and JOC Synopses.** For a Perspective, a black and white head-and-shoulders photograph and a very brief (one or two sentence) statement of the corresponding author’s current research interests should be included in a new section with the boldfaced heading **Author Information** located immediately before the Acknowledgments. For a JOC Synopsis, a black and white photograph and statement should be furnished for each coauthor. Model release and copyright forms are required for author photographs. They will be provided by the Journal office.

### 2.5.2 Color

The editors encourage the use of color in the table of contents/abstract graphic, and in individual manuscript graphics to enhance the clarity of presentation.

### 2.5.3 Quality

Because the graphics inserted into the manuscript are used for production, the quality of the graphics published in the Journal depends on the quality of the graphic images provided by authors. *Chemical structure graphics and figures can be moved and rescaled by the Journal production staff if necessary, but they cannot be otherwise modified or enhanced to correct problems or to improve their appearance.*

For uniformity of appearance, all the graphics of the same type, such as chemical structures, graphs, and spectra, should share a common graphic style and a common lettering font and size. Lettering and lines should be of uniform density. Arial or Helvetica font is preferred for lettering; the size should be at least 5.0 points. Lines should be no thinner than 1.0 point.

Digital graphics in the manuscript should have the following minimum resolution:

- Black-and-white line art: 1200 dots per inch (dpi)
- Grayscale art: 600 dpi
- Color art (RGB): 300 dpi

For graphics in the supporting information, a resolution of 300 dpi is usually adequate.

Photographs and other continuous-tone graphics should have high contrast. Manuscripts containing graphics with inadequate resolution or other quality problems may be delayed in manuscript evaluation or Journal production.

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

### 2.5.4 Chemical Structure Graphics

**Structures** are chemical structural formula line drawings used in schemes, equations, and structure blocks. A scheme depicts, with multiple reaction arrows, a series of chemical transformations among several structures. It may have vertical and diagonal as well as horizontal arrows, is identified with a sequential Arabic boldface numeral, and may have a short descriptive title (for example, **SCHEME 2. Synthesis of 10**). The scheme number and optional title are positioned above the scheme and should be typed at the appropriate location in the manuscript text word-processor file, not in the graphics program used to create the scheme. Each scheme must be referred to by its number at least once in the manuscript text. No collected list of all the scheme titles should be included at the end of the manuscript.

In reaction schemes, abbreviations for reagents, solvents, and reaction conditions should be placed above
the horizontal reaction arrows or adjacent to the vertical arrows; only if there is insufficient space should they be placed in footnotes below the scheme (with the footnotes typed into the manuscript text file and keyed to lowercase letters placed above or next to the arrows). It is not necessary to indicate reagents, solvents, and reaction conditions in detail since this information will be available in the experimental section or in a cited reference.

An equation illustrates simpler transformations with structures and horizontal reaction arrows in a single line, or expresses a relationship among mathematical or physical quantities. It is identified with a sequential Arabic numeral in parentheses flush with the right margin, has no title or footnotes, and is cited at least once in the text with “eq” followed by the numeral.

A structure block is a group of chemical structures that are placed together for efficient use of space. Structure blocks have neither numbers nor titles, and the structures are not connected with reaction arrows.


Structures should be produced with a drawing program such as ChemDraw or ChemBioDraw. Authors will find the necessary formatting parameters incorporated as the “ACS Document 1996” option in the Apply Document Settings menu. In ChemDraw Preferences, “cm” should be chosen as the units, and the tolerance should be set at 3 pixels. Authors using other drawing programs should select settings as close as possible to the following:

**Drawing Settings**
- **chain angle**: 120°
- **bond spacing**: 18% of length
- **fixed length**: 14.4 pt (0.508 cm, 0.2 in.)
- **bold width**: 2.0 pt (0.071 cm, 0.0278 in.)
- **line width**: 0.6 pt (0.021 cm, 0.0084 in.)
- **margin width**: 1.6 pt (0.056 cm, 0.0222 in.)
- **hash spacing**: 2.5 pt (0.088 cm, 0.0347 in.)

**Text Settings**
- **font**: Arial or Helvetica
- **size**: 10 pt

**Layout.** Chemical structure graphics should be inserted into the manuscript near their first mention in the text. Structures, arrows, and structure numbers should be arranged to make maximum use of the available one- or two-column width, and to occupy the minimum height necessary. During production of the PDF version of the paper, only one-column-wide structure blocks and equations are placed between paragraphs of text; schemes, and all two-column-wide graphics, are generally placed at the top of a column or page. In the HTML version, thumbnail links to the individual graphics are inserted after the paragraph in which each is first mentioned.

**Labeling of Structures.** Within structure blocks, equations, and schemes, the individual structures should be numbered with boldface Arabic numerals (“structure numbers”), in Arial or Helvetica font, in the order in which the compounds are first mentioned in the text. Structure numbers are also bolded where they appear in the text and in tables. To avoid the need to repeat similar structures, boldface lowercase letters may be used immediately following the numerals (for example, 5a, 5b) to distinguish variants that differ only in the identity of substituents (indicated in the structures with R^1, R^2, X, etc.). Where needed, numbers such as ring position indicators or NMR chemical shifts, or other markings such as double-headed arrows showing NOE correlations, may be included in structures.
2.5.5 Table of Contents/Abstract Graphic

A graphic must be included in each manuscript that will appear (1) in the table of contents (TOC) of the Journal issue in which the paper is published; (2) in the published paper immediately above the abstract; and (3) in any list of search hits generated on the ACS Publications Web site that includes the paper. This graphic should capture the reader’s attention and, in conjunction with the manuscript’s title, should give the reader a quick visual impression of the type of chemistry described in the paper. The TOC/Abstract graphic should not exactly duplicate a graphic appearing within the text of the manuscript. In this Journal the graphic is not accompanied by any caption or explanatory text.

Structures in the TOC graphic should be constructed as specified in section 2.5.4. Annotations should be limited to labels for compounds and reaction arrows. The use of standard abbreviations and unambiguous molecular formulas for common substituents, reagents, and solvents is encouraged. Nonstandard abbreviations should not be used in the graphic unless they are defined in the abstract. The TOC/Abstract graphic should be inserted immediately above the abstract on the first page of the manuscript file. It should not be uploaded as a separate file. The TOC graphic must be entirely original artwork created by one of the coauthors. It should not include a photograph, drawing, or caricature of any person, living or deceased. Copyrighted images should not be incorporated. Further guidance on creating the TOC graphic is available at http://pubs.acs.org/paragonplus/submission/toc_abstract_graphics_guidelines.pdf.

2.6 Supporting Information for Publication

All tables, graphics, and discussion that are peripheral or supplementary to the material in the manuscript file’s Results and Discussion section should be placed in the supporting information. Tables of yield optimization data, short descriptions of peripheral experiments immediately followed by a table, graph, or spectrum showing the results (for example, a kinetic isotope effect study), chemical assay procedures and data (including preparation of derivatives for analysis), bioassay procedures and data, computational methods and data, and X-ray crystallographic methods and data may be included in the supporting information.

A wide range of electronic formats is supported; a complete list can be found on the Paragon Plus Web site at http://pubs.acs.org/page/4authors/submission/software.html. They include formats for color illustrations, spreadsheets, rotatable molecular models, animations, and videos.

All supplementary text and graphics should be combined into a single PDF (preferred) or word-processor file. During submission, files submitted in word-processor format will be automatically converted to PDF files for posting on the ACS Publications Web server. If the file is furnished in word-processor format, page breaks should be inserted to separate items intended to appear on adjoining pages. If this is not done, captions for spectra and other graphics may not end up on the same page as the respective graphics in the PDF file created by Paragon Plus. If submission as a single file is not possible, then all files of the same file type should be combined. If more than one supporting information file is provided, the individual files should be given informative file names (for example, NMR_spectra.pdf and Additional_tables.doc). Authors should not upload numerous image files each containing a single spectrum or chromatogram. Crystallographic Information Framework (CIF) files should be uploaded separately from other types of files.

Text in the supporting information should be formatted in the same manner as the manuscript text (see section 2.3.4). The graphics must meet the same standards as the graphics in the manuscript (section 2.5) except that the resolution should not exceed 300 dpi. Spectra should be in sharp focus and have dark unbroken lines. Images generated by the spectrometer data-processing software are preferred over scanned images of printouts. For the convenience of reviewers and readers, it is preferred that pages with spectra be rotated to landscape orientation. Spectra and chromatograms should be labeled with a structure number (or table-entry number) and a small graphic of the structure. Axis labels and scales, peak frequencies or chemical shifts, and other text and numerical information must be clearly legible. If the manuscript reports the preparation of a compound under more than one set of experimental conditions, the
spectrum’s labeling or caption must indicate which conditions produced the sample whose spectrum is
illustrated. NMR spectra should be at least half-page in size, and the solvent and instrument frequency
should be indicated on each spectrum or in the caption. Column headings in tables, and axis labels in
spectra and graphs, must be in English. Tables, and graphics other than spectra and chromatograms,
should be numbered as in the following examples: Table S2; Figure S3. Informative captions for figures
other than spectra should appear directly below the figures. There are no restrictions on the use of color in
supporting information graphics.

All the pages of supporting information files containing text and graphics must be consecutively
numbered. The first page should be a title page with the title of the manuscript and the names of the
authors. If the file contains more than a single type of data (for example, copies of both NMR spectra and
chromatograms), include a table of contents for the file on the second page. If there is more than one file
submitted as Supporting Information, each file should have its own title page and table of contents.

Authors may furnish as supporting information a single compressed folder containing NMR free
induction decay (FID) data for selected compounds. The individual data files should be organized into
subfolders whose file names identify the compound (by the structure number used in the manuscript),
nucleus, and type of measurement. The data for each experiment should include a file with information
about data acquisition and processing parameters. An additional file in PDF (preferred) or Microsoft
Word format should serve as an index for the entire archive; it should display the structures and structure
numbers of all the compounds with FID data, and should identify the files’ formats and required software.
The index file and the subfolders containing the FID files should be combined into a single folder. That
folder should be ZIP-compressed, and the resulting file, with a "zip" file extension, should be uploaded
as an additional supporting information for publication file.

The supporting information is not copyedited during Journal production and will appear on the archival
Web server as submitted. Authors should be aware that references that are included in the supporting
information are not indexed by Web of Science (Science Citation Index).

2.7 Web Enhanced Objects

A Web enhanced object (WEO) is a graphic, spreadsheet, or multimedia file of supplementary data that
needs to be hyperlinked to a particular location in the manuscript text. A list of WEO file formats
compatible with Paragon Plus can be found on the Paragon Plus Web site at
http://pubs.acs.org/page/4authors/submission/woe.html. Files in other formats can be ZIP-compressed. At
the intended location for the link, the author should type the instruction “[Insert link to <WEO’s file
name> here]”. If specialized software is required to open a WEO, appropriate guidance should be
furnished in an endnote. When the manuscript is submitted through the Paragon Plus Web site, each WEO
should be uploaded with ‘Web Enhanced Object’ selected as the file designation. WEOs may not replace
or duplicate required supporting information, and they should not be mentioned in the supporting
information availability statement.

3 Submitting the Manuscript

3.1 Using the Paragon Plus Web Site

The manuscript and other submission items should be uploaded at ACS Paragon Plus. The Journal will
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Before submitting a manuscript, the corresponding author (or a designee who will be making the
submission) must register on the Paragon Plus Web site. Once registered, an author may submit
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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 Paragon Plus
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.

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The original version of the manuscript word-processor file is deleted from Paragon Plus when an editor requests a revision. It is therefore important for the author to retain a copy of this file when the manuscript is first submitted.

3.2 Additional Items to be Submitted

All manuscript files except for the cover letter are uploaded in step 5 of the submission process. The names of all files uploaded on the Paragon Plus Web site should include a file extension (e.g., "doc" or "docx" or "pdf"), even if the manuscript is created and submitted on a non-Windows computer. As each file is uploaded, the appropriate file designation (for example, ‘Compound Characterization Checklist’, ‘Supporting Information for Publication’, ‘Supporting Information for Review Only’, or ‘Other files for Editors only’) should be selected from the File Designation pull-down menu on the file-upload Web page. No file designation is needed for the cover letter, which is uploaded separately.

3.2.1 Cover Letter

A cover letter must accompany every manuscript. The cover letter should include the corresponding author’s name, postal and e-mail addresses, and telephone and fax numbers; the title of the manuscript; and a brief paragraph pointing out the significance of the reported work.

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. A copy of the report and any associated supporting information must be uploaded as supporting information for review only (see section 3.2.3).

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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 faxed or e-mailed to the editor as soon as it becomes available.

3.2.2 Compound Characterization Checklist

It is strongly encouraged that manuscripts are accompanied by a Compound Characterization Checklist when reporting the characterization of new compounds, known compounds that have been prepared by new or modified methods, or that present the results of theoretical computations. The Checklist will be provided to the reviewers to help them assess the overall thoroughness of the characterization of compounds and the reporting of computational results.

The Checklist form is available as a Microsoft Excel file on the Paragon Plus Web site at http://pubs.acs.org/page/joceah/submission/authors.html – select the Compound Characterization Checklist link. The form should be completed on-screen and saved with a “.xls” or “.xlsx” file extension. Alternatively, the version of the form included in section 5 of these Guidelines may be printed, completed by hand, scanned, and the image file saved with an appropriate file extension.

3.2.3 Supporting Information for Review Only

If the manuscript is an extension of a published or “in press” (accepted for publication) letter or communication, a copy of the preliminary report and any supporting information associated with it must be uploaded as a supporting information for review only file. When related work is cited but is not available to editors and reviewers because it is “submitted for publication” or “in press”, a copy of the cited manuscript should be provided in this manner. When an author requests back-to-back publication of related manuscripts submitted at the same time, each manuscript should include a copy of the companion paper as supporting information for review only. Renaming review-only files to indicate their relationship to the manuscript (for example, incorporating the reference number of a cited preliminary report or “in press” paper) will be helpful to reviewers and editors.

Authors may upload as supporting information for review only files any additional material not intended for publication that they wish the editors and reviewers to see. Files with copies of spectra and chromatograms, and Crystallographic Information Framework (CIF) files, should be uploaded as supporting information for publication, not as supporting information for review only.

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When revising a manuscript (or submitting a manuscript considered by another journal that was revised to address that journal's reviewer comments), author should use highlighting or Microsoft Word’s Track Changes tool to prepare an additional copy showing changes made. That copy should be uploaded as Other files for Editors only. (The file uploaded as the Manuscript File, and the Manuscript PDF file if one is furnished, must not contain highlighting, comments, or visible Track Changes edits.)

Any other material the author wishes the editor but not the reviewers to see should be uploaded as Other files for Editors only.

3.2.5 Journal Publishing Agreement

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Author should use highlighting or Microsoft Word’s Track Changes tool to prepare an additional copy showing changes made. That copy should be uploaded as Other files for Editors only. The revised word-processor file uploaded as the Manuscript File (and the Manuscript PDF file, if one is furnished) must not contain comments, colored text (including colored reference citation numbers), or color-highlighted text. **If the word processor’s Track Changes tool has been used, all changes must be accepted (incorporated as final) before that file is saved and uploaded.** Because the word-processor and PDF versions need to be identical, authors who furnish a PDF version of the revised manuscript text file should not further edit the word-processor or TeX/LaTeX version after the PDF version has been created. Authors who choose to have their accepted manuscripts published online as [Just Accepted](#) manuscripts (section 1.8.2) are strongly encouraged to furnish the revised manuscript in both PDF and word-processor versions.

The revision must be uploaded on the Paragon Plus Web site as a revised submission. New or replacement supporting information files can be added during revision; any files that are being replaced with updated versions should be removed. If any supporting information for publication is being added to a manuscript that previously had none, a supporting information availability statement (see section 2.1.11) must be added to the manuscript text file. Changes to the manuscript and to the supporting information, whether or not made in response to the reviewer and editor comments, should be pointed out in the “Response to Decision Letter” section of the revision-submission Web page. Any change in the manuscript’s title, abstract, or list of coauthors must be indicated. A new Journal Publishing Agreement (section 3.2.5) is required if there is a change of title or coauthors. If compound characterization data have been added or removed, or if the numbering of the reported compounds has changed, the Compound Characterization Checklist (section 3.2.2) should be replaced with an updated version.

If the first revision requested following peer review is not submitted within 30 days for an Article, Note, or JOCSynopsis, and the author has not made alternative arrangements with the editor for completion of the revision, the manuscript will be rejected. If an additional revision of an Article, Note, or JOCSynopsis is needed, the time limit will not be more than 14 days.

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via a secure Web site. Authors will access the secure site through ACS ChemWorx and will need an ACS ID. To obtain an ACS ID or to reset your password, go to www.acschemworx.org.

The author should return a detailed list of any needed corrections. Only typographic corrections and other minor changes may be made in a manuscript at the page proof stage. Any substantive changes will require editorial approval and may delay publication.

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guidance from the Committee on Publication Ethics (COPE) when considering retractions.

3.8 Additional Help

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# 4 Standard Abbreviations and Acronyms

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>α</td>
<td>observed optical rotation in degrees</td>
</tr>
<tr>
<td>[α]</td>
<td>specific rotation [expressed without units; the units, (deg·mL)/(g·dm), are understood]</td>
</tr>
<tr>
<td>Å</td>
<td>angstrom(s)</td>
</tr>
<tr>
<td>Ac</td>
<td>acetyl</td>
</tr>
<tr>
<td>acac</td>
<td>acetylacetonate</td>
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<tr>
<td>ADP</td>
<td>adenosine 5′-diphosphate</td>
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<tr>
<td>AIBN</td>
<td>2,2′-azobisisobutyronitrile</td>
</tr>
<tr>
<td>AMP</td>
<td>adenosine 5′-monophosphate</td>
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<tr>
<td>Anal.</td>
<td>combustion elemental analysis</td>
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<td>anhyd</td>
<td>anhydrous</td>
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<td>AO</td>
<td>atomic orbital</td>
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<td>aryl</td>
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<td>atm</td>
<td>atmosphere(s)</td>
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<td>ATP</td>
<td>adenosine 5′-triphosphate</td>
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<td>ATPase</td>
<td>adenosinetriphosphatase</td>
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<td>av</td>
<td>average</td>
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<td>9-BBN</td>
<td>9-borabicyclo[3.3.1]nonyl</td>
</tr>
<tr>
<td>9-BBN–H</td>
<td>9-borabicyclo[3.3.1]nonane</td>
</tr>
<tr>
<td>BINOL</td>
<td>1,1′-bi-2-naphthol</td>
</tr>
<tr>
<td>Bn</td>
<td>benzyl</td>
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<tr>
<td>BOC, Boc</td>
<td>tert-butoxycarbonyl</td>
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<tr>
<td>BODIPY</td>
<td>dipyrromethene boron difluoride</td>
</tr>
<tr>
<td>bp</td>
<td>boiling point, base pair</td>
</tr>
<tr>
<td>bpy</td>
<td>2,2′-bipyridyl</td>
</tr>
<tr>
<td>br</td>
<td>broad (spectral)</td>
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<tr>
<td>Bu, n-Bu</td>
<td>normal (primary) butyl</td>
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<td>s-Bu</td>
<td>sec-butyl</td>
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<td>t-Bu</td>
<td>tert-butyl</td>
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<td>Bz</td>
<td>benzyol (not benzyl)</td>
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<tr>
<td>B3LYP</td>
<td>3-parameter hybrid Becke exchange/Lee–Yang–Parr correlation functional</td>
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<td>°C</td>
<td>degrees Celsius</td>
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<td>calcld</td>
<td>calculated</td>
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<tr>
<td>cAMP</td>
<td>adenosine cyclic 3′,5′-phosphate</td>
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<td>CAN</td>
<td>ceric ammonium nitrate</td>
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<td>CASSCF</td>
<td>complete active space self-consistent field</td>
</tr>
<tr>
<td>CASPT2</td>
<td>complete active space with second-order perturbation theory</td>
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<td>cat</td>
<td>catalytic</td>
</tr>
<tr>
<td>CBZ, Cbz</td>
<td>benzyloxycarbonyl (preferred over the abbreviation Z)</td>
</tr>
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<td>CC</td>
<td>coupled cluster</td>
</tr>
<tr>
<td>CD</td>
<td>circular dichroism</td>
</tr>
<tr>
<td>cDNA</td>
<td>complementary deoxyribonucleic acid</td>
</tr>
<tr>
<td>CI</td>
<td>chemical ionization; configuration interaction</td>
</tr>
<tr>
<td>CIDNP</td>
<td>chemically induced dynamic nuclear polarization</td>
</tr>
<tr>
<td>CIF</td>
<td>Crystallographic Information</td>
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<td>centimeter(s)</td>
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<td>cm⁻¹</td>
<td>wavenumber(s)</td>
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<td>compd</td>
<td>compound</td>
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<td>concn</td>
<td>concentration</td>
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<td>correlation spectroscopy</td>
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<td>cyclopentadienyl</td>
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<td>m-CPBA</td>
<td>meta-chloroperoxybenzoic acid</td>
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<td>CV</td>
<td>cyclic voltammetry</td>
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<tr>
<td>Cy</td>
<td>cyclohexyl</td>
</tr>
<tr>
<td>δ</td>
<td>chemical shift in parts per million downfield from tetramethylsilane</td>
</tr>
<tr>
<td>d</td>
<td>day(s); doublet (spectral); deci density</td>
</tr>
<tr>
<td>DABCO</td>
<td>1,4-diazabicyclo[2.2.2]octane</td>
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<td>dansyl</td>
<td>5-(dimethylamino)-1-naphthalenesulfonyl</td>
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<td>DCM</td>
<td>dichloromethane</td>
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The Journal of Organic Chemistry

COMPOUND CHARACTERIZATION CHECKLIST

Corresponding Author ________________________________

1. Please print this Checklist form and complete the form by hand.
2. Enter the name of the corresponding author and the title of the manuscript above. For a revision or resubmission, enter the manuscript ID number next to "jo".
3. In the left-most column, enter the identifying numbers (or table-entry numbers) of the compounds or structures for which data are reported. Do not include known compounds prepared by literature methods or obtained from commercial sources. List them in the sequence in which they appear in the experimental section. For each compound, type a single "X" in either the "New" or the "Known" column.
4. For each compound or structure, place a single "X" in the columns corresponding to types of data reported in the experimental section and supporting information. You may use unlabeled columns for data types not listed. For most new compounds, the data should include HRMS or elemental analysis, and copies of 1H and 13C NMR spectra.
5. Scan the completed Checklist, and save the scanned image(s) with file names that include the appropriate file extension (.pdf or .jpg), even on a non-Windows computer.
6. Upload the saved file when submitting the manuscript. Select "Compound Characterization Checklist" as the file designation.

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Manuscript Title ________________________________
## Compound Characterization Checklist

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(* SI = Supporting Information)