JOC

The Journal of Organic Chemistry

Guidelines for Authors

Updated January 2016

REMINDER ABOUT SOME IMPORTANT MANUSCRIPT SUBMISSION REQUIREMENTS

Notes, Brief Communications, and *JOC*Synopses have **length limits**. The abstract, introductory remarks, and results and discussion of a Note do not exceed 3000 words; the limit for a Brief Communication is 2000 words. For Notes and Brief Communications, tables and graphics (figures, reaction schemes, and chemical structure graphics) are counted against 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. There are no word-count limits on the experimental section. For information about the length limit for *JOC*Synopses see section 2.3.3.

There are limits on the **number of references and explanatory endnotes** in Brief Communications (25) and *JOC*Synopses (80).

All **experimental procedures and compound characterization data** are included in the manuscript's experimental section. None appear in the supporting information, which is intended primarily for spectra, chromatograms, crystallographic data, documentation of theoretical calculations, and peripheral discussion.

All **tables and graphics** (figures, reaction schemes, and chemical structures) are inserted within the manuscript text where they are first discussed.

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.

When single-crystal X-ray diffraction structures are reported, **CIF files** are furnished as supporting information files, even if the data have been deposited in a crystallographic database.

A previous submission of substantially the same manuscript to any ACS journal is disclosed in the cover letter. If the submission was reviewed, the cover letter includes the reviews and a detailed explanation of the changes made in response to them.

The **names and contact information of all coauthors** are entered in step 2 of the manuscript submission process in the same sequence and form in which they appear on the manuscript.

CONTENTS – Section titles are clickable links

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 3.3.4).

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. They differ from letters or communications in not presenting preliminary results that the author intends to publish later in a more complete form. 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.

Brief Communications are short accounts of preliminary results of unusual novelty and urgency that justify immediate disclosure. They receive expedited processing by the editorial office, the reviewers, and the Journal production office. The length of a Brief Communication is limited to 2000 words, exclusive of the experimental section and the list of references and endnotes.

For both Notes and Brief Communications, 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). *JOC*Synopses 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.

Recent Reviews are bibliographic listings of review articles and specialized monographs that are prepared by the Journal's Recent Reviews Editor.

1.3 Manuscript Requirements

Manuscripts should be submitted on the American Chemical Society (ACS) Paragon Plus Web site at http://acs.manuscriptcentral.com/acs. This Web site and its online manuscript submission environment are referred to as Paragon Plus throughout these Guidelines.

A manuscript submitted to *The Journal of Organic Chemistry* must be based on original research by the authors. The originality of a submitted manuscript may be jeopardized, and the manuscript precluded from consideration for publication, if it contains "new" information that has been made publicly available, either in print or electronic format. Such disclosure includes posting of conference presentations, posters, and preprints on institutional repositories and other Web sites. 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. 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.

A Brief Communication is intended to be a preliminary disclosure and is published with the expectation that the study will subsequently be expanded and reported as a full paper in this or another journal. Because the requirements for urgency and novelty are very similar for Brief Communications and for papers published by *Organic Letters*, a manuscript previously declined by *Organic Letters* will not be considered for publication as a *JOC* Brief Communication.

Because a Brief Communication is a preliminary report and a *JOC* Note is an account of a completed study of limited scope, a rejected Brief Communication may not be resubmitted as a Note.

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, as well as 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 (section 3.3.1) 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. In addition, Brief Communications are evaluated against the criterion of urgency. 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, whether or not it was sent to reviewers, 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

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

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

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

1.6 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, in addition, 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 is published with each manuscript. During the submission process, the corresponding author must provide this statement on behalf of all authors of the manuscript and will be asked to select funding sources from the list of agencies included in the FundRef Registry http://www.crossref.org/fundref/. 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."

The editors wish to promote a community of authors and reviewers who participate and reciprocate in the development of knowledge. Authors who submit manuscripts to the Journal may be asked from time to time to review manuscripts submitted by other researchers. Authors who repeatedly decline requests to review for the Journal or renege on commitments to review may be asked to submit their future manuscripts to other journals.

1.7 Online Publication

The Journal is published biweekly in printed and online editions.

1.7.1 Articles ASAP

The copyedited final versions of accepted papers are published as *Articles ASAP* (As Soon As Publishable) on the Journal's 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.xxxxxxx is assigned to each accepted manuscript. Authors are given instructions for citing their work by DOI in an e-mail communication 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.

1.7.2 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. No supporting information or Web enhanced object files are included with a *Just Accepted* manuscript. During the manuscript submission process, an author can choose to have the manuscript posted online as 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 3.7). 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.

1.8 Cover Art

The cover of each printed issue of the Journal, and the table of contents page of each online issue, feature author-submitted artwork, often a computer-generated graphic or a graphic–photograph montage, that is related to an Article or Perspective in that issue. The editors encourage authors to submit imaginative artwork that highlights an aspect of the work being reported. Submissions should measure 7 in. (18 cm) wide by 8 in. (20 cm) high, should have a minimum resolution of 300 dpi, and should be saved in TIFF or EPS format. Additional information about preparing cover art may be obtained from the Editor-in-Chief's office (e-mail: joc@chem.utah.edu). Artwork prepared for consideration as cover art should be e-mailed to the Editor-in-Chief after receipt of the related manuscript has been acknowledged.

2 Preparing the Manuscript and Supporting Information

2.1 Manuscript Organization

The sections of a manuscript are:

- Title
- Authors' names and addresses
- Corresponding author's e-mail address
- Table of Contents/Abstract Graphic
- Abstract
- Introduction
- Results and Discussion [may be separate]
- Conclusion [optional]
- Experimental Section [except Perspectives, *JOC*Synopses, and accounts of purely theoretical studies]
- Acknowledgments [optional]
- Supporting Information availability statement [required if the manuscript is accompanied by any supporting information for publication]
- References and Endnotes

***Section Headings*.** The only section headings used in a Note or Brief Communication are **Experimental Section, Acknowledgments,** and **Supporting Information.** An Article has, in addition, **Introduction, Results and Discussion,** and **Conclusion** section headings. A *JOC*Synopsis has the same section headings as a Note except that there is no Experimental Section.

2.1.1 Title

The title should accurately, clearly, and concisely identify the subject and emphasis of the reported work. The wording of the title is important for current awareness alerts and for information retrieval. 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.

During manuscript submission, the submitting author must enter contact information for *all* of the coauthors (see section 3.1). Because these author names are automatically imported into the electronic Journal Publishing Agreement (section 3.3.6), and into the cover page and table-of-contents page entry for the optional *Just Accepted* manuscript (section 1.7.2), the names must be entered into Paragon Plus in the same sequence, and in exactly the same form, as they appear on the first page of the manuscript. If author names and contact information are automatically imported from existing Paragon Plus registration data by entering e-mail addresses of the coauthors, the names should be checked against those on the first page of the manuscript file to ensure they are identical, particularly with regard to the presence or absence of a middle name or middle initial.

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 2.5.7.

2.1.5 Abstract

The abstract for an Article, Note, or Brief Communication 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 *JOC*Synopsis or Perspective, the abstract should identify the scope and focus of the manuscript. The length of the abstract for a Note, Brief Communication, or *JOC*Synopsis 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 not be used in the abstract.

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 introduction of an Article should require no more than two double-spaced manuscript pages. The opening paragraph of a Note, Brief Communication, or *JOC*Synopsis 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, Brief Communication, or *JOC*Synopsis.

Authors are encouraged to make use of ***supporting information for publication***, which is supplementary material that is submitted at the same time as the manuscript and is linked to the published paper on the Journal Web site. The use of supporting information is particularly appropriate for presenting additional discussion, graphs, spectra, and tables that are more likely to be of interest to specialists than to general readers, but *all* experimental procedures and compound characterization data must appear in the manuscript's experimental section (section 2.1.9), not in the supporting information. Individual items in the supporting information can be cited in the discussion by referring to their table or figure numbers. Section 2.6 ('Supporting Information') discusses the mechanics of preparing this material for submission. Unless otherwise stated, the term "supporting information" in these Guidelines refers to this type of supplementary material and not to "supporting information for review only" (see section 3.3.4).

2.1.8 Conclusion

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

2.1.9 Experimental Section

Every manuscript reporting the results of experimental work must include an experimental section. This section should describe experimental methods in sufficient detail to permit repetition of the work by others. For a Note, Brief Communication, or Article, *all* the experimental procedures and listings of compound characterization data, and any associated literature citations, must be included in the manuscript file's experimental section. 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.

Special attention should be called to hazardous compounds or operations, and appropriate precautions should be described.

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. It should be placed in the manuscript file 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, any 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.

Manufacturers and model names or numbers of spectrometers, chromatographs, polarimeters, X-ray diffractometers, and other standard laboratory instruments should not be identified. Commercial and institutional providers of analytical and spectrometric services (or the institutional affiliations of instrument facilities) should not be named.

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, but the manufacturer should not be identified unless that manufacturer donated the instrument. Authors whose cover art submissions are used may later add a recognition of the graphic artist.

2.1.11 Supporting Information Statement

If the manuscript is accompanied by any supporting information for publication, a brief list of the types of data included in this supplementary material is required in the manuscript. The list entries need not be detailed, but they should be more specific than "spectra" or "additional tables". "Experimental procedures" and "compound characterization data" will not appear here, since *JOC* requires experimental procedures and characterization data listings to be placed in the manuscript file's experimental section. The appropriate format is:

> **Supporting Information.** Brief statement in nonsentence format listing the contents of the material supplied as supporting information.

The manuscript cannot be forwarded for publication if this statement is missing. During production of the accepted manuscript, the Supporting Information statement will be incorporated into the 'Associated Content' section of the published paper.

2.1.12 References and Endnotes

All the references and any explanatory notes must be combined into a single consecutively numbered list at the end of the manuscript text. The references and endnotes should be numbered with Arabic numerals in the order of their first citation in the text, and the corresponding citation numbers should be inserted at the appropriate locations in the text as superscripted numerals without parentheses or brackets. 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 ([4a–f]). In the PDF and HTML versions of the published paper, the references and endnotes will appear grouped together at the end of the text. In both versions, many of the references will have links to the 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 their 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 most recent ones should be cited; if appropriate, the author may add “and references cited therein” following a reference. Any articles, communications, letters, patents, theses, and conference abstracts in which portions of the reported work have been previously disclosed must be cited. 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 *JOC*Synopsis. No reference should repeat or cite 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; remarks that require illustration with graphic structures or reaction schemes should be incorporated into the discussion or placed in the supporting information. See section 2.3.3 for limits on the number of references and endnotes allowed in Brief Communications and *JOC*Synopses.

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. 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. Digital Object Identifier (DOI) numbers should be furnished for papers published online too recently to have 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 the uniform resource locator (URL). References to Web pages and documents on personal, research group, and departmental Web sites should be avoided because their long-term availability cannot be assured.

2.2 Specialized Data

Data needed to document structure assignments, purity assessments, and other conclusions should be included in the manuscript and supporting information. Referencing a link to an author's Web page or to an institutional depository, or stating that data will be provided to readers upon request, is not an acceptable alternative.

2.2.1 Synthesis Experiments

Synthesis procedures for new compounds should be accompanied by listings of the most important product characterization data. 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, Brief Communications, and Articles, *all* experimental procedures and listings of compound characterization data must be included in the manuscript file's 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 the next fully characterized bold-titled compound.

Reactant, reagent, and catalyst quantities should be given in both weight and molar units. Reaction solvent volumes should be reported. Use of standard abbreviations (see 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.

Yields reported in experimental examples, and yields presented in the discussion for comparison with alternative or previously reported synthetic methods, should represent weighed amounts of isolated and purified products. Yields of products should be reported in the experimental section as both weights and percentages.

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

Manuscripts that illustrate a new or modified synthetic method with multiple examples conducted on a submillimolar scale should include one or more examples carried out on a larger scale 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.

Reports of syntheses conducted in microwave reactors must clearly indicate whether sealed or open reaction vessels were used and must document the manufacturer and model of the reactor, the method of monitoring the reaction mixture temperature (external surface sensor or internal probe type), and the temperature reached or maintained in each experiment. Reporting a wattage rating or power setting is not an acceptable alternative to providing temperature data. 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.

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 by the reported preparation, isolation, and purification methods. 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 the attained purity be documented compound-by-compound, either qualitatively with copies of spectra or chromatograms, or numerically with 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 (1) report the yields (as both weights and percentages); (2) cite the published characterization data that have been compared with the data obtained for the synthesized compounds (this requirement cannot be met by furnishing CAS registry numbers); and (3) 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 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 3.3.2) 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 a required type of data is not obtainable (for example, a compound that is too insoluble to record a carbon NMR spectrum, or too unstable to obtain a good elemental analysis), 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 $^{13}C\{^{1}H\}$ for proton-decoupled carbon data. Proton NMR shifts, reported to 0.01 ppm precision, should be accompanied by an abbreviation for any multiplet structure, the number of atoms represented by the peak or multiplet, and coupling constants where applicable. Carbon NMR peak shifts should be rounded off to the nearest 0.1 ppm except when greater precision is needed to distinguish closely spaced peaks. Information about numbers of attached hydrogen atoms (reported as C, CH, CH_2, CH_3) from DEPT, DEPTQ, PENDANT, or 2D spectra may be included with the carbon peak shifts. 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 being interleaved in a single list. For the 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 proton 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 images of the spectra should be high enough to allow the fine structure of multiplets to 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, unconsumed reactants, and incompletely removed extraction, chromatography, or recrystallization solvents). Peak suppression may be used on the NMR solvent peak for samples run in protic solvents, but it is never necessary for samples run in deuterated solvents.

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.

The 'Publishing Tools' page on the ACS Publications Web site has a link to additional guidance for reporting NMR data in research papers.

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 supporting information availability statement (see section 2.1.11). Copies of the frequency-domain spectra are required whether or not FID data are provided.

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 (historically called 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 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 mixture cannot be separated into its components, it is usually acceptable to report elemental analysis or HRMS data for the mixture. Elemental analysis or HMRS 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.

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 (if present) 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, TOF, quadrupole, or ion trap) should be reported. The *ACS Style Guide* format for reporting accurate mass data is: HRMS (ESI-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 $[\alpha] = (100 \cdot \alpha)/(l \cdot c)$ should be reported as unitless numbers as in the following example: $[\alpha]_D^{20}$ –25 (*c* 1.9, $CHCl_3$), where the concentration *c* is in g/l00 mL and the path length *l* is in decimeters. The units of the specific rotation, (deg·mL)/(g·dm), are implicit and are not included with the reported value.

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).

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 (see ‘Identity’ above).
- 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 necessarily depend on the method of preparation, the compound's air and thermal stability, the complexity of its structure, the nature of reasonably likely impurities, and the amount of sample available. For example, combustion analysis would not be an appropriate choice for the product of an isomerization reaction; and NMR methods would not be appropriate when reasonably likely impurities (including unreacted starting materials) do not have unique resonances or are NMR-silent (for example, an inorganic salt). 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 2.5.6), 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. Since a thermal ellipsoid plot is required in the supporting information (see below), there is no need to include a ball-and-stick drawing or thermal ellipsoid plot in the manuscript file unless specific features of the structure are being addressed in the discussion.

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.

Regardless of the level of detail of the discussion of the structure, a Crystallographic Information Framework (CIF) file containing complete details of data collection, crystal and unit-cell parameters, structure solution and refinement, and tables of atomic coordinates and thermal parameters, bond lengths, bond angles, and torsion angles must be furnished as Supporting Information for Publication. Reflection intensity data (structure factor tables) are not required. If more than one crystal structure is being reported, the individual CIF files should be combined and uploaded as a single supporting information file. *The CIF files are required whether or not the data have been deposited in a crystallographic database*.

CIF files should be saved in text-only (plain ASCII) format and should be assigned file names that identify the structure numbers 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. Any reported syntax errors 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, *not* as Supporting Information for Publication.

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. The inclusion of these data should be confirmed on the **Compound Characterization Checklist** (see section 3.3.2). 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 extend to development of new bioassay methods, it is expected that any reported bioassay data will have been collected following a cited method, so that a detailed description of the test protocol is not required. If alterations in the test method have been made, that fact should be clearly noted where the results are presented, and the modified protocol should be described in detail in the supporting information.

Regardless of whether a standard or modified method is used, the description of the bioassay 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 purity level of at least 95% needs to be documented.

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 may want professional assistance with improving the English, figures, or formatting in their manuscript before submission. ACS ChemWorx Authoring Services can save time and improve the communication of research in the manuscript. More information about the services offered is available at http://es.acschemworx.acs.org. Manuscripts with extensive English usage or grammar deficiencies will not be forwarded to reviewers.

2.3.2 Word-Processor and PDF Versions

The author's manuscript word-processor or TeX/LaTeX file is used (after revision, if needed) for Journal production. The manuscript file is provided to the reviewers in both a portable document format (PDF) version and a HTML version. 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. [Only a single version of any supporting information files should be submitted; see section 2.6]. Additional information about author-supplied manuscript PDF files is available at http://pubs.acs.org/page/4authors/submission/file_upload.html. 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. The length of a Brief Communication is limited to 2000 words for the abstract, introductory paragraph, and the results and discussion. Authors may use the word-count tool in Microsoft Word for checking adherence to these limits. 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 *JOC*Synopsis 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 25 for a Brief Communication and 80 for a *JOC*Synopsis. 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 at http://pubs.acs.org/page/4authors/submission/software.html. 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.

Fonts and Typography. Times, Times New Roman, Helvetica, Arial, or Courier fonts (12-point size is preferred) 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 (rather than the normal text 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 in 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 manuscript PDF file. [Pages in supporting information files (see section 2.6) are not automatically numbered by Paragon Plus and do need to be numbered by the author.]

Formatting and Page-Size Setting. This Journal does not require the use of a manuscript template and does not provide journal-specific templates. For any type of submission, the entire manuscript file, including the abstract, the experimental section, and the references and endnotes must be formatted as **single-column, double-spaced text**. Authors should not try to simulate the formatting and appearance of copyedited published Journal papers. Automatic hyphenation should be disabled, and line returns ("Return" or "Enter" key) should be used only at the end of paragraphs and section headings, and where tables and graphics are inserted. The paper-size setting in the word processor's Page Setup menu should be set to U.S. Letter (8.5 × 11 in., 22 × 28 cm). If A4 or another setting is used, lines of text may be lost when an editor or reviewer prints the PDF file on U.S. letter-size paper.

Placement of Tables and Graphics. All tables (see section 2.4) and graphics (see section 2.5) 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. When saving the manuscript file, the file format should not be changed from the word processor's default document file type. The file name should include a file extension (".doc" or "docx" for Word; ".wpd" for WordPerfect), even if the manuscript is created on a non-Windows computer. 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 (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 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 of these Guidelines. 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. 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 CH_3 or Me may be used for "methyl", but not both.

Symbols for physical quantities should be italicized (for example, *c*, E_a, *J*, *m/z*, $t_{1/2}$). 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

The use of tables is encouraged for presenting data in a space-efficient manner. **Tables must be inserted in the manuscript word-processor file near their first mention in the text**; they should not be grouped together at the end of 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 and Brief Communications, 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 (illustrations) 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; they should not be grouped together at the end of the text. 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 and Brief Communications (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.

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 3.3.1).

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 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. Although there is no charge for inclusion of color illustrations in the manuscript, paper reprints (see section 3.6) containing color graphics have a supplemental color charge of $100 per 100 copies. There are no restrictions on the use of color in the supporting information. In selecting colors for illustrations, authors should keep in mind that many readers will print the published paper on monochrome printers or will receive black-and-white copies from document providers.

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

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.

For graphics in the *supporting information*, a resolution of 300 dpi is usually adequate. 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 Inserting Graphics into the Manuscript

For manuscripts created with a word-processor program, each graphic should be copied from the source program and pasted near its first mention in the manuscript text file. To allow pasted graphics to be positioned without overlapping nearby text, Microsoft Word users may need to select "In line with text" as the text-wrapping style. If a pasted graphic needs to be resized or relabeled, it should be re-edited in the source program or with a graphics processor, and the resized image pasted again into the word-processor file (rather than modified within the word-processor program). *No page-layout or graphics-placement instructions should be typed into the text file*.

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.

2.5.5 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 linked with reaction arrows.

Formatting. The drawing and annotation of individual structures should follow IUPAC recommendations for graphical representation of chemical structure diagrams (http://www.iupac.org/publications/pac/80/2/0277/pdf/). The manner of indicating out-of-plane orientation of substituents and rings should adhere to IUPAC recommendations for graphical representation of stereochemical configuration (http://www.iupac.org/publications/pac/2006/pdf/7810x1897.pdf).

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.

2.5.6 Figures

Diagrams, graphs, spectra, photographs, and all other types of illustrations are presented in the Journal as figures with captions. Blocks of structures and reaction schemes should not be designated as figures. Figures should be inserted into the manuscript 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.

Figures are consecutively numbered with boldface Arabic numerals and have brief descriptive captions. The figure number and caption should be typed in the manuscript word-processor file directly *below* the figure (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.

2.5.7 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 2.5.5 ('Chemical Structure Graphics'). 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 on the Web at http://pubs.acs.org/paragonplus/submission/toc_abstract_graphics_guidelines.pdf.

2.6 Supporting Information

Where the term "supporting information" is used without further qualification in these Guidelines, it refers to files of supplementary material that are linked to the published paper (supporting information for publication) and not to supporting information for review only (section 3.3.4). The technical content of the supporting information is discussed in several sections above: 2.1.7 ('Results and Discussion'), 2.1.9 ('Experimental Section'), and 2.2 ('Specialized Data'). This section describes the mechanics of preparing the supporting information for submission. Authors are reminded that descriptions of experimental procedures, and listings of compound characterization data, must not be placed in the supporting information but should be included in the manuscript file's experimental section. The only exceptions are that 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. Therefore, *authors should not submit both word-processor and PDF versions of the same supporting information file.* 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. Incorporating images created or saved at resolutions higher than 300 dpi will not substantially improve the appearance of graphics in the Web-based supporting information but will result in large file sizes that may inconvenience reviewers, editors, and future readers with long download times. 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 both 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; in many cases this can be accomplished by providing a table-entry number. 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), a table of contents for the file, with the page numbers on which each type of data begins, should be included on the first page. If there is more than one file, each file should have its own title page and table of contents. The requirements for numbering the pages and for providing a title page with a table of contents apply only to supporting information files furnished in word-processor or PDF format.

Authors may optionally 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 exactly as submitted. Authors should be aware that references that are included in the supporting information but not in the manuscript are not indexed by *Web of Science (Science Citation Index)*.

A supporting information availability statement identifying the type of supplementary material being furnished must be inserted in the text of the manuscript immediately after the acknowledgments (see section 2.1.11). *The manuscript cannot be forwarded for publication if this statement is missing* when one or more files of supporting information for publication has been provided.

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/weo.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 (see section 3.3) should be uploaded at the ACS Paragon Plus Web site at http://acs.manuscriptcentral.com/acs. The Journal cannot consider manuscripts received by e-mail.

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 manuscripts to any ACS journal and may check the processing status of submitted manuscripts. Registration is not required to access information about preparing and submitting manuscripts. The Web site's security features limit access to a submitted manuscript to the editorial offices and to those reviewers to whom that manuscript is assigned.

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

Submitting authors have the option to provide existing ORCID iDs for coauthors during submission, but they cannot create new ORCID iDs for coauthors.

During step 2 of the submission process, the submitting author must enter contact information for *all* of the coauthors. For a coauthor who is already registered as an author or reviewer in Paragon Plus, this can be done automatically by entering the coauthor's registered e-mail address and clicking the "Find" button. Coauthors are not required to register. Because these author names are automatically imported into the electronic Journal Publishing Agreement (section 3.3.6), and into the cover page and table-of-contents page entry for the optional *Just Accepted* manuscript (section 1.7.2), the names must be entered into Paragon Plus in the same sequence, and in exactly the same form, as they appear on the first page of the manuscript.

During step 3 of the submission process, authors are required to enter the names and e-mail addresses of at least five researchers qualified to act as reviewers.

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 Priority Processing

Manuscripts that are complete and that adhere to the requirements in these Guidelines will receive priority for processing by the Editor-in-Chief's office and for assignment to an associate editor. The specific requirements that need to be met to qualify for priority processing are listed in the box on the next page titled Priority Processing Requirements. If any of those requirements are not met, the author of an Article, Note, or *JOC*Synopsis will be given 14 days (two to seven days for a Brief Communication, depending on the revisions needed) to furnish a completed or corrected resubmission. *The "Received" date will be*

changed to the date on which the complete, corrected submission is received in the Editor-in-Chief's office.

3.3 Additional Items to be Submitted

All manuscript files except for the cover letter (see below) 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 (for example, ".doc" or "docx" for Microsoft Word, or ".pdf" for Portable Document Format), even if the manuscript is created and submitted on a non-Windows computer. Reviewers and editors will be able to see the file names assigned by authors (although manuscript and supporting information file names will get replaced with system-generated numerical file names when the manuscript is published). 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 from the other submission files.

3.3.1 Cover Letter

A cover letter must accompany every manuscript. It is either typed, copied-and-pasted, or attached as a file in step 4 of the submission process. 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 3.3.4).

Previous Submission. If substantially the same manuscript has been previously submitted to this or another ACS journal, whether or not it was sent to reviewers, the cover letter must mention the earlier submission. If the manuscript was reviewed, copies of all of the reviews should be appended to the cover letter file or uploaded as 'Other files for Editors only' (see section 3.3.5), and the cover letter should include a detailed explanation of any revisions, whether or not they were made in response to reviewer and editor comments.

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

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

The permission letter or message should be appended to the cover letter file or uploaded as 'Other files for Editors only' (see section 3.3.5). 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.

Priority Processing Requirements

To qualify for priority in the initial processing and assignment to an associate editor, a manuscript for an Article, Note, Brief Communication, or *JOC*Synopsis needs to meet the minimum formatting and completeness requirements listed below. Most of these requirements have been established to facilitate the job of the reviewers and editors. ***Evaluation of a manuscript not meeting these requirements will be delayed while the Journal office requests a corrected submission prior to review.*** The manuscript will be assigned a new "Received" date when the resubmission is received.

Manuscript Submission Web Form

- The names of all the coauthors are entered in step 2 in the same sequence and form as they appear on the first page of the manuscript.

Manuscript File

- For a Note, Brief Communication, or *JOC*Synopsis, the word-count and reference-count limits are not exceeded.
- The entire manuscript is formatted as single-column, double-spaced text.
- The references and endnotes are grouped into a single list at the end of the manuscript file.
- The manuscript's graphics and tables are inserted into the text near their first mention. They are not grouped together at the end of the manuscript or, except for TeX/LaTeX submissions, uploaded as separate files.
- The manuscript and supporting information files are free of font and graphics-quality problems.
- The manuscript does not have extensive English usage or grammar deficiencies.
- For new compounds, required data, including **either** MS accurate mass or elemental analysis data, **and both** proton and carbon NMR data, are furnished in the experimental section.

Supporting Information for Publication

- Required data (including images of NMR spectra for new compounds; purity data for known compounds prepared by new or modified methods; and copies of Crystallographic Information Framework files) are furnished.
- Images of NMR spectra are combined into a single supporting information file (or a small number of such files); they are not uploaded as numerous separate image files. Spectra and their axis labels are easily legible.

Supporting Information for Review Only

- A copy of any published preliminary report, including any supplementary material associated with it, is uploaded as a supporting information for review only file, and the report is mentioned in the cover letter and cited in the manuscript's introductory remarks.
- A copy of any cited "in press" or "submitted-for-publication" paper is provided as a supporting information for review only file.

Other

- Any previous submission of substantially the same manuscript to this or another ACS journal is disclosed in the cover letter. Copies of the reviews are appended to the cover letter or uploaded as "Other files for Editors only". The cover letter identifies in detail the changes made in response to reviewer and editor comments.
- A Compound Characterization Checklist is furnished if the manuscript reports the characterization of new compounds or known compounds prepared by a new or modified method.

There are additional less critical manuscript preparation and submission requirements that are listed in these Guidelines. Authors of manuscripts that qualify for priority processing will be asked to bring their manuscripts into compliance with these secondary requirements following peer review.

3.3.2 Compound Characterization Checklist

Manuscripts that report the characterization of new compounds or known compounds that have been prepared by new or modified methods, or that present the results of theoretical computations, must be accompanied by a completed Compound Characterization Checklist. 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.

3.3.3 Supporting Information for Publication

The technical content of the supporting information is discussed in sections 2.1.7 ('Results and Discussion'), 2.1.9 ('Experimental Section'), and 2.2 ('Specialized Data'). The formatting of the supporting information is discussed in section 2.6 ('Supporting Information').

3.3.4 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.

3.3.5 Other Files For Editors Only

When revising a manuscript (including a new submission that was previously considered by another journal and subsequently revised to address that journal's reviewer comments), the author should use highlighting or Microsoft Word's Track Changes tool to prepare an additional copy showing the 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.

3.3.6 Journal Publishing Agreement

A properly completed and signed Journal Publishing Agreement must be submitted for each manuscript. ACS Paragon Plus provides an electronic version of the Agreement that will be available on the **My Authoring Activity** tab of the corresponding author's Home page once the manuscript has been assigned to an editor. A PDF version of the Agreement that is prepared and uploaded at the time of manuscript

submission is also available. **Authors are strongly encouraged to use the electronic Journal Publishing Agreement**. If the PDF version is used, **all pages of the signed form must be submitted**. If the corresponding author cannot or should not complete either the electronic or PDF version for any reason, another author should complete and sign the PDF version of the form. Forms and complete instructions are available at http://pubs.acs.org/page/copyright/journals/index.html.

If a manuscript is not accepted for publication or is withdrawn, the transfer of the copyright to the ACS included in the Journal Publishing Agreement is automatically canceled.

The supporting information for publication associated with an accepted and published manuscript is considered part of the publication and is covered by the copyright assignment in the Journal Publishing Agreement. Material in the supporting information should not be presented as new data in a future paper.

3.4 Revising the Manuscript

In revising a manuscript following peer review and editor evaluation, the author should address any concerns raised by the reviewers. If substantial changes need to be made in content or interpretation, it is appropriate for the author to obtain the concurrence of the other coauthors. Requests for changes or additional data noted in the editor's letter should also be accommodated. *For a Note, Brief Communication, or JOCSynopsis, the changes must be made without exceeding the word-count limits* (section 2.3.3). The revision should be rechecked for consistent notation and for sequential numbering of structures, schemes, equations, figures, tables, and references. References should be reverified, and the status of any "submitted for publication" and "in press" manuscripts, and of any references cited as online pre-publications (*Articles ASAP* for ACS journals) at the time of the original submission, should be updated.

When revising a manuscript, the author should use highlighting or Microsoft Word's Track Changes tool to prepare an additional copy showing the changes that have been 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 be password-protected and 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 1.7.2) 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, **not as a new manuscript**. It may not be submitted by e-mail. 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 3.3.6) 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 3.3.2) 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 *JOC*Synopsis, or 15 days for a Brief Communication, 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 *JOC*Synopsis is needed, the time limit will not be more than

14 days. Because of the rapid turnaround time at each stage of processing, a Brief Communication judged by the editor to require more than minor changes will be rejected rather than returned to the author for revision.

3.5 Page Proofs

The page proofs for an accepted and copyedited manuscript, and a reprint order form, will be provided to the corresponding author 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.

3.6 E-prints and Reprints

Under the ACS Articles on Request policy, the Society will provide (free of charge) to corresponding authors a unique URL within the ACS Web site that they may e-mail to colleagues or post on external Web sites. These author-directed links are designed to facilitate distribution of an author's published work to interested colleagues. The ACS Articles on Request policy allows 50 downloads within the first year after publication and unlimited access via the same author-directed link 12 months after publication.

ACS AuthorChoice options establish fee-based mechanisms for authors or their research funding agencies to sponsor the open availability of final published articles on the Web. *ACS AuthorChoice* offers authors a wide range of open access license options, such as Creative Commons licenses and provisions for immediate or 12-month embargoed open access, and includes ACS Certified Deposit. Authors will find useful information about compliance with open access policies available here and FAQs here. Corresponding authors who published with ACS during 2014 may have access to *ACS Author Rewards*, a $60M stimulus program ACS provided to help authors transition to new open access publishing models.

After acceptance, authors will be presented with the opportunity to purchase an *ACS AuthorChoice* option, and authors who do so will be presented with the appropriate license at that time. For a review of all license options available, see here. For questions or further assistance with *ACS AuthorChoice*, please reach out to support@services.acs.org.

When authors are sent the proof of their paper, they will receive a link to a Web site where they may order hardcopy (paper) reprints. They may also call Cierant Corporation (866-305-0111) from 9AM to 5PM EST. Reprints will be shipped within two weeks after the issue publication date. Neither the editors nor the Washington ACS Office keeps a supply of reprints; requests for single copies of papers should be addressed to the corresponding author of the paper concerned.

3.7 Additions and Corrections

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4 Standard Abbreviations and Acronyms

α	observed optical rotation in degrees
[α]	specific rotation [expressed without units; the units, (deg·mL)/(g·dm), are understood]
Å	angstrom(s)
Ac	acetyl
acac	acetylacetonate
ADP	adenosine 5′-diphosphate
AIBN	2,2′-azobisisobutyronitrile
AMP	adenosine 5′-monophosphate
Anal.	combustion elemental analysis
anhyd	anhydrous
AO	atomic orbital
aq	aqueous
Ar	aryl
atm	atmosphere(s)
ATP	adenosine 5′-triphosphate
ATPase	adenosinetriphosphatase
av	average
9-BBN	9-borabicyclo[3.3.1]nonyl
9-BBN–H	9-borabicyclo[3.3.1]nonane
BINOL	1,1′-bi-2-naphthol
Bn	benzyl
BOC, Boc	*tert*-butoxycarbonyl
BODIPY	dipyrromethene boron difluoride
bp	boiling point, base pair
bpy	2,2′-bipyridyl
br	broad (spectral)
Bu, *n*-Bu	normal (primary) butyl
s-Bu	*sec*-butyl
t-Bu	*tert*-butyl
Bz	benzoyl (not benzyl)
B3LYP	3-parameter hybrid Becke exchange/ Lee–Yang–Parr correlation functional
°C	degrees Celsius
calcd	calculated
cAMP	adenosine cyclic 3′,5′-phosphate
CAN	ceric ammonium nitrate
CASSCF	complete active space self-consistent field
CASPT2	complete active space with second-order perturbation theory
cat	catalytic
CBZ, Cbz	benzyloxycarbonyl (preferred over the abbreviation Z)
CC	coupled cluster
CD	circular dichroism
cDNA	complementary deoxyribonucleic acid
CI	chemical ionization; configuration interaction
CIDNP	chemically induced dynamic nuclear polarization
CIF	Crystallographic Information Framework
cm	centimeter(s)
cm^{-1}	wavenumber(s)
compd	compound
concd	concentrated
concn	concentration
COSY	correlation spectroscopy
Cp	cyclopentadienyl
m-CPBA	*meta*-chloroperoxybenzoic acid
CV	cyclic voltammetry
Cy	cyclohexyl
δ	chemical shift in parts per million downfield from tetramethylsilane
d	day(s); doublet (spectral); deci
d	density
DABCO	1,4-diazabicyclo[2.2.2]octane
dansyl	5-(dimethylamino)-1-naphthalenesulfonyl
DBN	1,5-diazabicyclo[4.3.0]non-5-ene
DBU	1,8-diazabicyclo[5.4.0]undec-7-ene
DCC	*N*,*N*′-dicyclohexylcarbodiimide
DCE	1,2-dichloroethane
DCM	dichloromethane
DDQ	2,3-dichloro-5,6-dicyano-1,4-benzoquinone
DEAD	diethyl azodicarboxylate
DEPT	distortionless enhancement by polarization transfer
DFT	density functional theory
DIBALH	diisobutylaluminum hydride
DMA	dimethylacetamide
DMAP	4-(*N*,*N*-dimethylamino)pyridine
DMDO	dimethyldioxirane
DME	1,2-dimethoxyethane
DMF	dimethylformamide
DMPU	1,3-dimethyl-3,4,5,6-tetrahydro-2(1*H*)-pyrimidinone
DMSO	dimethyl sulfoxide
DMT	4,4′-dimethoxytrityl (4,4′-dimethoxyltriphenylmethyl)
DNA	deoxyribonucleic acid
DPS	*tert*-butyldiphenylsilyl
dr	diastereomer ratio
DTT	dithiothreitol
E1	unimolecular elimination
E2	bimolecular elimination
EA	ethyl acetate
ED_{50}	dose effective in 50% of test subjects

EDTA	ethylenediaminetetraacetic acid
EI	electron impact
EPR	electron paramagnetic resonance
eq	equation
equiv	equivalent
er	enantiomer ratio
ESI	electrospray ionization
Et	ethyl
FAB	fast atom bombardment
FD	field desorption
FID	flame ionization detector; free induction decay
Fmoc	9-fluorenylmethoxycarbonyl
FT	Fourier transform
g	gram(s); prefix to NMR abbreviation denoting gradient-selected (e.g. gCOSY, gHMQC)
GC	gas chromatography
GTP	guanosine 5′-triphosphate
h	hour(s)
HF	Hartree–Fock
HMBC	heteronuclear multiple bond correlation
HMPA	hexamethylphosphoric triamide (hexamethylphosphoramide)
HMQC	heteronuclear multiple quantum correlation
HOMO	highest occupied molecular orbital
HPLC	high-performance liquid chromatography
HRMS	high-resolution mass spectrometry
HSQC	heteronuclear single quantum correlation
Hz	hertz
ICR	ion cyclotron resonance
IP	ionization potential
IR	infrared
IRC	intrinsic reaction coordinate
J	coupling constant (in NMR spectrometry)
k	kilo
K	kelvin(s) (absolute temperature)
L	liter(s)
LAH	lithium aluminum hydride
LCAO	linear combination of atomic orbitals
LD_{50}	dose that is lethal in 50% of test subjects
LDA	lithium diisopropylamide; local density approximation
LFER	linear free energy relationship
LHMDS	lithium hexamethyldisilazane, lithium bis(trimethylsilyl)amide
lit.	literature value (abbreviation used with period)
LTMP	lithium 2,2,6,6-tetramethylpiperidide
LUMO	lowest unoccupied molecular orbital
μ	micro
m	multiplet (spectral); meter(s); milli
M	molar (moles per liter); mega
M^+	parent molecular ion
MALDI	matrix-assisted laser desorption ionization
max	maximum
MCD	magnetic circular dichroism
MCR	multicomponent reaction
MCSCF	multi-configuration self-consistent field
MD	molecular dynamics
Me	methyl
MEM	(2-methoxyethoxy)methyl
Mes	2,4,6-trimethylphenyl (mesityl) [not methylsulfonyl (mesyl)]
MHz	megahertz
min	minute(s); minimum
mM	millimolar (millimoles per liter)
MM	molecular mechanics/modeling
MO	molecular orbital
mol	mole(s); molecular (as in mol wt)
MOM	methoxymethyl
mp	melting point
MRCI	multi-reference configuration interaction
mRNA	messenger ribonucleic acid
Ms	methylsulfonyl (mesyl)
MS	mass spectrometry
MTBE	methyl *tert*-butyl ether
MW, mol wt	molecular weight
m/*z*	mass-to-charge ratio (not *m*/*e*)
N	normal (equivalents per liter)
NAD^+	nicotinamide adenine dinucleotide
NADH	reduced NAD
NBO	natural bond orbital
NBS	*N*-bromosuccinimide
NCS	*N*-chlorosuccinimide
NHC	N-heterocyclic carbene
NICS	nucleus-independent chemical shift
NIS	*N*-iodosuccinimide
nm	nanometer(s)
NMO	*N*-methylmorpholine-*N*-oxide
NMP	*N*-methylpyrrolidone
NMR	nuclear magnetic resonance
NOE	nuclear Overhauser effect
NOESY	nuclear Overhauser effect spectroscopy
NRT	natural resonance theory
Nu	nucleophile
OD	optical density
ORD	optical rotary dispersion
PCC	pyridinium chlorochromate
PDC	pyridinium dichromate
PE	petroleum ether
PES	photoelectron spectroscopy
Ph	phenyl
piv	pivaloyl
pm	picometer(s)
PMB	*p*-methoxybenzyl
PPA	poly(phosphoric acid)
ppm	part(s) per million

Pr	propyl
*i*Pr	isopropyl
PTC	phase-transfer catalysis
py	pyridine
q	quartet (spectral)
QM	quantum mechanics
QSAR	quantitative structure–activity relationship
RCM	ring-closure metathesis
redox	reduction–oxidation
rel	relative
R_f	retention factor (in chromatography)
RHF	restricted Hartree–Fock
ROESY	rotating frame Overhauser effect spectroscopy
ROMP	ring-opening metathesis polymerization
rRNA	ribosomal ribonucleic acid
rt	room temperature
s	singlet (spectral); second(s)
SAR	structure–activity relationship
SCF	self-consistent field
SEM	scanning electron microscopy; 2-trimethylsilylethoxymethyl
SET	single electron transfer
S_N1	unimolecular nucleophilic substitution
S_N2	bimolecular nucleophilic substitution
S_N'	nucleophilic substitution with allylic rearrangement
SOMO	single-occupied molecular orbital
t	triplet (spectral)
t	time; temperature in units of degrees Celsius (°C)
T	absolute temperature in units of kelvins (K)
TBAB	tetrabutylammonium bromide
TBAC	tetrabutylammonium chloride
TBAF	tetrabutylammonium fluoride
TBS	*tert*-butyldimethylsilyl
TBHP	*tert*-butyl hydroperoxide
TCA	trichloroacetic acid
TCNE	tetracyanoethylene
TDDFT	time-dependent density functional theory
TEAB	tetraethylammonium bromide
temp	temperature
TEMPO	2,2,6,6-tetramethylpiperidin-1-oxyl
TES	triethylsilyl
Tf	trifluoromethanesulfonyl (triflyl)
TFA	trifluoroacetic acid
TFAA	trifluoroacetic anhydride
THF	tetrahydrofuran
THP	tetrahydropyran-2-yl
TIPS	triisopropylsilyl
TLC	thin-layer chromatography
TMAI	tetramethylammonium iodide
TMEDA	*N*,*N*,*N*′,*N*′-tetramethyl-1,2-ethylenediamine
TMS	trimethylsilyl; tetramethylsilane
TOF	time-of-flight; turnover frequency
TON	turnover number
Tr	triphenylmethyl (trityl)
tRNA	transfer ribonucleic acid
t_R	retention time (in chromatography)
Ts	*para*-toluenesulfonyl (tosyl)
TS	transition state
UHF	unrestricted Hartree–Fock
UV	ultraviolet
VCD	vibrational circular dichroism
vis	visible
vol	volume
v/v	volume per unit volume (volume-to-volume ratio)
wt	weight
w/w	weight per unit weight (weight-to-weight ratio)

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COMPOUND CHARACTERIZATION CHECKLIST

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Corresponding Author _____

Manuscript Title _____

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.
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COMPOUND			IDENTITY													PURITY					COMPUTATIONAL DATA IN SI*			AUTHOR REMARKS
Compound, structure, or table-entry number	New	Known	Known made by new/modified method	Weight and percentage yield	Physical state / mp range if cryst. solid	IR	UV-Vis	1H NMR	13C NMR	MS	MS Accurate mass (HRMS)	Optical rotation/ORD/CD	Enantiomeric/Diastereomeric ratio	X-ray [ORTEP and CIF in SI*]	Copy of 1H/13C NMR spectrum in SI*	Copy of chromatogram in SI*	Quant GC, HPLC, electrophoresis	Elemental analysis		Cartesian coordinates or Z-matrix	# of imaginary frequencies	Total energy	(* SI = Supporting Information)

5. Compound Characterization Checklist

CONTINUATION SHEET

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COMPOUND CHARACTERIZATION CHECKLIST

Corresponding Author _____

COMPOUND			IDENTITY												PURITY					COMPUTATIONAL DATA in SI*			AUTHOR REMARKS
Compound, structure, or table-entry number	New	Known made by new/modified method	Weight and percentage yield	Physical state / mp range if cryst. solid	IR	UV-Vis	1H NMR	13C NMR	MS	MS Accurate mass (HRMS)	Optical rotation/ORD/CD	Enantiomeric/Diastereomeric ratio	X-ray [ORTEP and CIF in SI*]	Copy of 1H/13C NMR spectrum in SI*	Copy of chromatogram in SI*	Quant GC, HPLC, electrophoresis	Elemental analysis		Cartesian coordinates or Z-matrix	# of imaginary frequencies	Total energy	(* SI = Supporting Information)