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2015 Guidelines for Authors

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Changes for 2015

Spectra guidelines have been modified.

Section [3.17.2](#)

Added: Spectra files should not be manipulated in any manner that could result in misinterpretation or misrepresentation of the original spectra.

Section [3.17.3](#)

Added: All original primary NMR data (e.g. FID files) supporting a submission should be retained and provided if requested.

1. Scope and Editorial Policy

Organic Letters invites original reports of fundamental research in all branches of the theory and practice of organic, physical organic, organometallic, medicinal, and bioorganic chemistry. In the selection of manuscripts for publication, the Editors place emphasis on the quality, originality and wide interest of the work.

The purpose of *Organic Letters* is rapid disclosure of the key elements of significant studies that are of interest to a large portion of the organic community. Authors should provide enough background information to place the new disclosure in context and to justify the rapid publication format. Full details should be reserved for an Article, which should appear in due course.

Manuscripts should be submitted online on the secure American Chemical Society (ACS) Paragon Plus Web site at <http://paragonplus.acs.org/login>. Hardcopy submissions are not considered. The length of a Letter can be 2, 3, or 4 pages, and back-to-back Letters will be considered. Use of color, when warranted, will be offered at no cost to authors.

Submission of a manuscript to the Journal implies that the work reported therein has not been previously published and is not under consideration for publication elsewhere in any medium, including preprints, electronic journals, and computer databases of a public nature. Submission also implies that all authors listed have agreed to publication of the material submitted.

1.1 Scope Details

One-step organic transformations must be highly innovative. For designed structures, if the design, synthesis and spectral data of a new compound are not

exceptionally novel, then data such as biological, binding, or materials properties should be included to justify the significance of the manuscript. Novel organic electronic materials need to illustrate either a novel synthetic method or interesting device properties.

Submissions regarding analytical detection of a selected species must contain a novel synthetic protocol and/or demonstrate notable improvement on the limits of detection of the species relative to contemporary protocols. The synthesis of a novel compound(s) or a significantly improved route to a known compound will only be considered, if appropriate improved device or use data is provided. A description of the synthesis of a known compound via known methods together with new sensing data falls outside the scope of Organic Letters and will not be considered, unless the new binding or sensing data provides a significant advance on previously reported selectivity and/or sensitivity for a target species and/or a novel mode of binding for a particular species under consideration.

1.2 Professional Ethics

Authors should adhere to the ACS Ethical Guidelines that are published periodically in this and other ACS journals and are available on the web at <http://pubs.acs.org/ethics/index.html>. Authors must inform the editor of related manuscripts that the author has published or has under editorial consideration or in press. Fragmentation of research reports should be avoided. Use of the text from another paper without direct quotation and attribution is plagiarism and comprises a serious violation of the ACS ethical guidelines. Use of text from an author's own previous paper comprises self-plagiarism. **Note: All ACS manuscripts are screened for plagiarism at revision.**

ACS Publications uses CrossCheck's iThenticate software to screen submitted manuscripts for similarity to published material. Further information about plagiarism can be found in Part B of [ACS Ethical Guidelines](#).

When submitting a manuscript to the Journal via ACS Paragon Plus, the submitting author is asked to identify the funding sources for the work presented in the manuscript. Identifying funding sources is optional during submission of an original manuscript. Funding source information is required when a revised manuscript is submitted. The authors should disclose at the time of submission all other potential sources of bias, including affiliations and financial or management relationships, that may constitute conflicts of interest. For further information, refer to the [ACS Ethical Guidelines](#) (see [2.2](#) for details on conflict of interest disclosures).

1.3 Peer Review

The Editor-in-Chief's office examines all manuscripts submitted. If a manuscript is ready to be reviewed, the corresponding author will be notified by email of the name and contact information of the Associate Editor. If a submission is incomplete or there are serious formatting deficiencies, the submission will be inactivated (see [2.4](#) for details on inactivation).

The Editors generally seek the advice of experts about manuscripts; however, manuscripts considered by the Editors to be inappropriate for *Organic Letters* or in violation of the ACS Ethical Guidelines may be rejected without review. The Editors, who accept full responsibility for decisions about manuscripts, may not always follow the recommendations of reviewers. The names of reviewers will not be given to authors without the consent of the reviewer. Authors should list the names of at least 5 persons competent to review their manuscripts (see [2.6.2](#) for details).

2. Submission of Manuscripts

Authors should submit manuscripts and accompanying materials via the Web at <http://paragonplus.acs.org/login>. All manuscripts must be formatted using the *Organic Letters* template (see [3.2](#) for details about the template). Directions and an overview of the electronic submission process are available at <http://pubs.acs.org/OrgLett>. Authors must also submit all revisions of manuscripts via the ACS Paragon Plus Environment. The web submission site employs state-of-the-art security mechanisms to ensure that all electronically submitted papers are secure. These same security mechanisms are also utilized throughout the peer-review process, permitting access only to editors and reviewers who are assigned to a particular paper. Authors needing assistance in submitting a manuscript via the web submission site should contact the Journal Help Desk (pubshelp@acs.org) or the Editor-in-Chief's office (eic@orglett.acs.org). Manuscripts submitted in hardcopy, as an email attachment, or by fax will not be considered.

2.1 Previously Submitted Work

Manuscripts previously rejected by *Organic Letters* must be submitted as new manuscripts. The authors should list in their cover letter the previous manuscript number, the previous *Organic Letters* Editor, a list of the changes made in the manuscript, and a rationale as to why the work should be reconsidered. Submissions without this information will be inactivated (see [2.4](#) for details on inactivation).

If substantially the same manuscript has been previously submitted to another ACS journal and declined, authors are requested to include, as part of the cover letter to *Organic Letters*: copies of the reviews, the ACS editor's decision letter, and, most

importantly, a detailed list of changes made to the manuscript, particularly changes made in response to reviewer comments. This information can facilitate evaluation of the paper. The Editor may accept the manuscript on the basis of the previous reviews and author remarks, may seek additional reviews, or may reject a paper without further review.

2.2 Conflict of Interest Disclosure

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. 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.”

2.3 Work Funded by NIH

Authors submitting publications describing research funded by the United States agency National Institutes of Health (NIH) should provide the normal Journal Publishing Agreement form at submission (see [2.6.3](#) for details on Journal Publishing Agreement forms). An NIH policy addendum form, which provides several options for compliance with NIH Public Access Policy, will be sent to authors whose papers have been accepted for publication. NOTE: This form will be sent from the Publications office, not the journal editor’s office. Information on complying with the NIH Public Access Policy Mandate, including a description of the compliance options available from ACS, is available at <http://pubs.acs.org/page/policy/nih/index.html>.

2.4 Inactivation of Incomplete or Incorrectly Formatted Submissions

The manuscript must be complete at time of submission and must conform to all formatting requirements (see [3](#) for details on preparing manuscripts). English usage and syntax must be acceptable. Required material, such as compound identity/purity documentation (see [4.3](#) for details on compound characterization) or information regarding prior submission of the work must be submitted (see [2.1](#) for details on prior submissions). If any of these criteria are not met, the submission will be inactivated and author will be asked to furnish the requested material or make the necessary changes. The receipt date will be changed to the date on which the complete, properly prepared submission is received.

2.5 Authors

Include as authors all those who have made substantial contributions to the work. Submission implies that all authors listed have agreed to publication of the material submitted and all have seen the submitted version of the work. Submission also implies that no person who has contributed to the work has been omitted. Single authors may be asked to verify that sole authorship is appropriate.

2.5.1 Corresponding Author (while manuscript is under review)

This is the (one) author to whom all correspondence will be sent while the manuscript is under consideration and to whom the proofs will be sent if the manuscript is accepted for publication, unless another author is specifically designated in the cover letter accompanying the submission. This author is assumed to have obtained permission to include all of the persons listed in the manuscript as authors, and assumes the responsibility of corresponding with all coauthors of the paper as to the progress of the paper.

2.5.2 Co-author Information

The author list should include all those who have made substantial contributions to the work. During manuscript submission, the submitting author must provide contact information (full name, email address, institutional affiliation and mailing address) for all of the co-authors. Because all of the author names are automatically imported into the electronic Journal Publishing Agreement, the names must be entered into ACS Paragon Plus in the same sequence as they appear on the first page of the manuscript. (Note that co-authors are not required to register in ACS Paragon Plus.) Deletion or addition of an author after the manuscript has been submitted requires confirming letters to the Editor-in-Chief (see [2.5.3 'Changes in Authorship'](#) for details). For more information on ethical responsibilities of authors, see the [ACS Ethical Guidelines](#).

2.5.2 Institution Address

The author affiliation(s) listed should be the institution(s) where the work was conducted. If the present address of an author differs from that at which the work was done, the current address should be given in a footnote.

2.5.3 Changes in Authorship

If any change in authorship is necessary after a manuscript has been submitted, **all authors (including any author added or deleted) must email the Editor assigned, confirming that they agree to the change.** If an author change is made at revision, the change should be noted in the revision cover letter, or in the 'Response to Decision Letter' section at the revision submission site, and all authors must email the Editor (as above).

2.5.4 Equal Authorship Designations

Simple equal authorship statements are allowed; itemization of individual author contributions or partial authorship is not permitted.

2.5.5 ORCID

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.

2.6 Items to be Submitted

In addition to the manuscript, the following items should be included where appropriate. NOTE: some items are required, e.g., the Cover Letter.

2.6.1 Cover Letter

A letter must accompany the manuscript. The postal address, telephone number, fax number, and email address of the author who should receive all correspondence concerning the manuscript during the evaluation period should be provided (see [2.5.1](#) ‘Corresponding Author’).

The letter should address the criteria of significance and the need for rapid disclosure and, if the author wishes, list the name of suggested Associate Editor(s) (Note: suggestions for Associate Editors will be considered, but may not be implemented based on an Editor’s schedule/manuscript load). Information regarding previous submission to *Organic Letters* or to any other ACS journal should be included (see [2.1](#) ‘Previously Submitted Work’). If back-to-back publication with another paper is desired, this should be stated, along with the desired order of publication in the cover letters of both manuscripts.

2.6.2 Reviewer Information

Authors should provide the names and email addresses of at least 5 recommended reviewers at section 3 of the Paragon Plus submission process: ‘Reviewers and Editors’. Ideally, these should be individuals who have published recently in the area of the paper. In the cover letter, authors may also request that certain individuals not be used as reviewers. Such a request will be honored by the Editor, unless it is believed that individual’s opinion is vital in the consideration of the manuscript

2.6.3 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 become 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 is also available, but **Authors are strongly encouraged to use the electronic Journal Publishing Agreement**. If the PDF version is used, **all pages of the signed PDF Agreement 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>.

2.6.4 Review-Only Material

Authors may include additional material not intended for publication that they wish Editors and reviewers to see. The first page should be marked “Review-Only Material”. The material should be uploaded with the file designation “Supporting Information for Review only”. NOTE: all experimental and characterization information submitted should be designated as ‘Supporting Information for Publication’ when it is uploaded into Paragon. (Any material the author wishes the editor *but not the* reviewers to see should either be appended to the cover letter file or uploaded as ‘Other files for Editors only’).

2.6.5 Unpublished References / Related Work

Authors are reminded that they must inform the editor of related manuscripts that the author has published or has under editorial consideration or in press. When references are cited and such work is not available to the referees because it is “in press” or has been submitted to this or other journals, this work should be submitted with the manuscript for use by the referees and the editors. These should be uploaded with the file designation “Supporting Information for Review only”.

2.6.6 Supporting Information

Given that the Editors are fully committed to providing the organic community with the most reliable and well-documented methods in the chemical literature, Supporting Information is required and is reviewed for completeness and accuracy by a Data Analyst. Compound characterization closely follows the guidelines of *The Journal of Organic Chemistry* (see [4](#) for experimental requirements and [3.17](#) for details on presenting Supporting Information). All experimental and characterization information submitted should be designated as ‘Supporting Information for Publication’ when it is uploaded into Paragon.

Supporting Information must be submitted at the same time as the manuscript and uploaded separately to the ACS Paragon Plus Environment. A [list of acceptable](#)

[file types](#) is available on the Web. Where possible, all Supporting Information files of the same type should be prepared as a single file (rather than submitting a series of files containing individual images or structures). For example, all Supporting Information available as PDF files should be contained in one PDF file.

DO NOT UPLOAD FIGURES AND TABLES THAT ARE TO BE PUBLISHED IN THE ARTICLE AS SUPPORTING INFORMATION FILES.

Submissions without adequate Supporting Information will be inactivated and the authors will be requested to provide the requested information. The receipt date for incomplete submissions will be changed to the date that all materials are received (see [3.17](#) 'Preparation of Manuscript: Supporting Information' and [4](#) 'Experimental Data Requirements' for details).

2.6.7 Compound Characterization Checklist (optional)

When manuscripts report the synthesis of compounds, submission of a completed Compound Characterization Checklist (CCC) is recommended *but not required*. The CCC form at <http://pubs.acs.org/page/orlef7/submission/ccc.html> can be completed on-screen and saved for uploading with the submission of the manuscript. The file should be uploaded with the file designation: 'Compound Characterization Checklist'. The CCC will be provided to reviewers to help them assess the overall thoroughness of the characterization of synthesized compounds.

3. Preparation of Manuscript

Authors should consult *The ACS Style Guide* (3rd ed., 2006, Oxford University Press, ISBN 0-8412-39999; <http://pubs.acs.org/books/>) for format guidance.

3.1 Word-Processor and PDF Versions of the Manuscript

The author's manuscript word-processor file is used (after revision, if needed) for Journal production. The manuscript file accessed by the reviewers is a portable document format (PDF) version of that file. Authors may either submit both versions, or they may submit only the word-processor version, and have Paragon Plus create the PDF for their inspection prior to the final step of manuscript submission (see [3.6](#) for details on preparing PDF files). Because the two versions need to be identical, no changes should be made to the word-processor file after the PDF version has been created.

3.2 Template

Organic Letters requires authors to prepare manuscripts using the template available on the Web. Use of the template will expedite publication, allow authors to indicate preferences for placement of artwork, and enable authors to determine whether their manuscript is within the 4-page limit. Manuscripts not formatted

using the template will be inactivated (see [2.4](#) for details on inactivation). The template is available in several word processing versions at the *Organic Letters* Web edition home page via <http://pubs.acs.org/OrgLett>. The ReadMe files at this URL provide details on how to prepare a manuscript using the template. The template should not be used to create an exact facsimile of a published manuscript. It can be used as a guide to indicate preferences for placement of artwork and to determine whether a manuscript is within the 4-page limit. (See [3.3](#) for details on published length versus length in the template.)

3.3 Manuscript Length

Published manuscripts can be no longer than 4 pages. Submissions which greatly exceed the 4-page limit will be inactivated.

3.4 Fonts

Authors should use only the fonts specified in the *Organic Letters* manuscript templates to prepare their manuscripts and Supporting Information. Arial or Helvetica font should be used for all text in schemes, figures, and structure blocks. To designate accents, the prime symbol, and the degree symbol, the Symbol fonts that came with an English language word processor should be used. NOTE: 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 Normal or Symbol font should be followed by the capital letter C in Normal font. The Symbol font set should also be used for Greek characters (rather than the 'basic Greek' subset of the normal font which is found in some word processors).

3.5 English Language

Any author who is not fully fluent in English is urged to obtain assistance with manuscript preparation from a technical editing service or a fluent colleague. The ACS ChemWorx English Editing Service can assist you in improving and polishing the language in your manuscript. You can learn more about the services offered, at <http://es.acschemworx.acs.org>. Manuscripts with extensive English language deficiencies will be inactivated (see [2.4](#) for details on inactivation).

3.6 PDF Preparation

Authors who create and submit their own PDF files should (1) use Adobe Distiller, not PDFWriter; (2) embed all fonts if possible; (3) check the PDF file before submission; and (4) print the file to check that all graphics and special characters such as Greek letters and degrees C appear correctly.

3.7 Title

Titles should clearly and concisely reflect the emphasis and content of the paper. Titles are of great importance for current awareness and information retrieval and

should be carefully constructed for these purposes. The use of abbreviations and acronyms in the title and abstract should be avoided. The same title should appear in the manuscript, the Supporting Information and in Paragon.

3.8 Author List

The author list in the manuscript should match the authors listed in Paragon at submission. To facilitate indexing and retrieval and for unique identification of an author, use first names, initials, and surnames (e.g., John R. Smith) or first initials, second names, and surnames (e.g., J. Robert Smith). At least one author must be designated with an asterisk as the person to whom correspondence should be addressed (see [2.5](#) for details on authors). Author list in the Supporting Information should match the list in the manuscript. If authors do not match, the manuscript will be inactivated. (see [2.4](#) for details on inactivation)

3.9 Table of Contents and Abstract Graphic

A single graphic which will be used for both the Table of Contents and Abstract must be supplied with each manuscript. **Do not include two versions of the graphic.** The graphic, in conjunction with the manuscript title, should give the reader a summary of the chemistry described in the paper. The graphic can be no wider than 9.0 cm and no taller than 3.5 cm and should be prepared following the specifications in [5](#) 'Artwork'. Text should be limited to the labeling of compounds, reaction arrows, and diagrams, with liberal use of R and X groups. Place the graphic at the beginning of the manuscript, just above the abstract. Do NOT include separate copies in the Supporting Information or with file designation 'Graphic for manuscript'

3.10 Abstract

All manuscripts must contain an abstract, not exceeding 75 words, which should briefly state the purpose of the research, the principal results, and major conclusions.

3.11 Text

Section headings such as Introduction, Conclusion, etc. should not be used. Letters do not contain a separate Experimental Section. Those data or procedures essential to the discussion and/or reproduction of the work should appear in the narrative, the footnotes, or in the Supporting Information.

3.11.1 Nomenclature

Registered trademark names should be capitalized whenever used. Trade and trivial names should not be capitalized. Usually the chemical name or composition should be given in parentheses or in a footnote at the first occurrence of such a name. *Chemical Abstracts (CA)* nomenclature rules are described in Appendix IV

of the *Chemical Abstracts Index Guide*. For CA nomenclature advice, consult the Manager of Nomenclature Services, Chemical Abstracts Service, P.O. Box 3012, Columbus, OH 43210-0012. A name generation service is available for a fee through CAS Client Services, 2540 Olentangy River Road, P.O. Box 3343, Columbus, OH 43210-0334; telephone (614) 447-3870; Telefax (614) 447-3747; or e-mail: answers@cas.org.

3.11.2 Abbreviations, Physical Quantity Symbols, and Units

Authors are encouraged to use abbreviations and acronyms to conserve space. A list of Standard Abbreviations and Acronyms is found in [Section 13](#) of these Guidelines. Consult also the *ACS Style Guide* (3rd ed., 2006, Oxford University Press, ISBN 0-8412-39999; <http://pubs.acs.org/books>) for additional information on abbreviations, symbols and units. Nonstandard abbreviations and acronyms must be defined the first time they are used in the abstract and in the text. The use of abbreviations should be consistent throughout the manuscript text and graphics. For example, either CH₃ or Me may be used for “methyl”, but not both.

3.12 References and Footnotes

Authors should ensure that they have identified and cited all relevant work that has influenced the current research. Authors should cite all of their own work that is related to the current submission, especially work that is currently under consideration at another journal. Cited work that has been submitted for publication (e.g., submitted; in press) must be provided to the Editor at submission. These manuscripts can be uploaded at submission with the file designation “Supporting Information for Review only”.

Unnecessarily long reference lists should be avoided. Literature citations and explanatory notes must be numbered, using Arabic numbers, in one consecutive series by order of appearance in the text, with the numbers presented as unparenthesized superscripts. Bibliographic references to classified documents and reports or to unpublished material not generally available to the scientific public should not be used. For reports published online, the DOI should be furnished in addition to the standard bibliographic information. Authors must obtain written permission from any person not listed as an author of the submission whose work is cited as a personal communication, unpublished work, or work in press.

Authors should consult *The ACS Style Guide* (3rd ed., 2006, Oxford University Press, ISBN 0-8412-39999; <http://pubs.acs.org/books>), for the appropriate style to use in citations. In literature references, journal abbreviations should be those used by *Chemical Abstracts* [see *Chemical Abstracts Service Source Index (CASSI) 1907-2004*]. The accuracy of the references is the responsibility of the authors. Because subscribers to the Web edition of the Journal are now able to click on the

“CAS” tag following each reference to retrieve the corresponding CAS abstract, reference accuracy is critical.

3.13 Schemes/Figures

See [5](#) ‘Artwork’ for instructions on drawing Schemes and Figures. Include reagents and conditions over reaction arrows in Schemes. Do not place conditions in Scheme legends. All Schemes/Figures/Tables should be included in the manuscript. Do NOT include separate copies in the Supporting Information or with file designation ‘Graphic for manuscript’.

3.14 Spectra in Manuscript

A brief summary of spectral data can be provided in the Letter as a footnote. Details should be provided as Supporting Information. Reproductions of spectra will be published in *Organic Letters* only when concise numerical summaries are inadequate for the discussion. Letters dealing primarily with 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 within the paper is essential, only the pertinent sections, prepared as figures should be presented. Spectra used as adjuncts to the characterization of compounds should be included as figures in the Supporting Information. (See [4](#): ‘Experimental Data Requirements’ for details on spectra required as Supporting Information and [3.17.2](#) for details on presenting spectra in Supporting Information.)

3.15 Tables

Tables should be numbered consecutively with Arabic numerals and should be placed within the text at the appropriate place. Each table should include a descriptive heading that, together with the individual column headings, makes the table self-explanatory. Column headings should be lower case, except for symbols and proper names. Text of column headings should not be bolded or italicized. Column headings should have a light gray background (choose gray 15% in Word), and no lines. Footnotes in tables should be given letter designations and be cited in the table by italic superscript letters. The sequence of letters should proceed by line rather than by column. If a reference is cited both in the text and in a table, a lettered footnote should be inserted in the table that refers to the numbered reference in the text. In setting up tabulations, authors are requested to keep in mind the type area of the journal page (17.8 in., 25.0 cm) and the column width (3.3 in., 8.5 cm) and to make tables conform to the limitations of these dimensions. When arranging data into columns, space should be used efficiently. Tables should be formatted to fill the column width.

3.16 Acknowledgment

The acknowledgment section can be used to provide information on funding sources and recognize contributions/assistance from colleagues. Provide an affiliation for all persons listed in the acknowledgment.

3.17 Supporting Information

The content of the Supporting Information is discussed in [4](#) ‘Experimental Data Requirements’. This section describes the criteria for presenting the Supporting Information for submission.

The Supporting Information format of this journal can accommodate many types of supplementary figures or data (e.g., reproductions of spectra, experimental procedures, tabulated data, expanded discussion of peripheral findings). Do not submit both word-processor and PDF versions of the same Supporting Information file. The author should include a Supporting Information Available statement at the end of the manuscript that describes this material. The appropriate format is **“Supporting Information Available: Brief statement in nonsentence format listing the contents of the material supplied as Supporting Information.”** Text in the Supporting Information should meet the same formatting and font requirements as the manuscript text. Graphics must meet the same quality standards as the graphics in the manuscript (see [3.14](#) ‘Spectra’ for requirements for spectra). Incorporating images in the Supporting Information created or saved at resolutions higher than 1200 dpi will not substantially improve the appearance of graphics but will result in large file sizes that inconvenience reviewers, editors, and future readers with long download times.

- the pages must be numbered (S1, S2 etc.) in ALL files
- manuscript title and authors should be listed on the first page (NOTE: If several files are submitted, author/title should be listed in EACH file)
- if the Supporting Information is extensive, a table of contents should be included The preferred method is to submit one file, embedding any graphics into a consolidated word processing file, rather than submitting a series of files containing individual images or structures. However:
- no one file should exceed 5 MB
- CIF information should be submitted as a separate file (see [3.17.4](#) for details on CIF files)

3.17.1 Experimental Section

An introductory section should include general procedures, standard techniques, and instruments employed in the synthesis and characterization of compounds described subsequently in this section. Special attention should be called to

hazardous reactions or toxic compounds. General reaction conditions should be described in the introductory section. Each procedure should include a title containing the compound number that corresponds to the manuscript, a chemical name or compound type, and structure. Procedures should be listed in numerical order. For synthetic procedures data should include: physical state and description, amount in weight or molar units, percent yield, and characterization data. Report ^1H chemical shift to two digits after the decimal point and ^{13}C chemical shifts to one digit after the decimal point, unless an additional digit will help distinguish overlapping peaks. (See [4](#) for experimental data requirements.)

3.17.2 Spectra

Standards for Spectra in the Supporting Information:

1. Spectra files should not be manipulated in any manner that could result in misinterpretation or misrepresentation of the original spectra.
2. Spectra should be at least a half page in size (Horizontal orientation is required)
3. Have dark unbroken lines
4. Label with a small graphic of the structure (using ChemDraw or related program) AND a compound number
5. Axis labels, scales, peak frequencies, chemical shifts and all other text or numerical information must be clearly legible on each spectra, and English characters must be used.
6. A caption should note the nucleus being measured, the solvent (formula preferred, e.g. C_6D_6 over benzene- d_6) and the field strength.
7. The field strength should be noted on each spectrum as well as in a comment in the general experimental section.
8. All peaks in the ^1H NMR should be integrated
9. Chemical shift values should be included
10. The largest peak in the ^1H NMR spectrum should normally be full scale and arise from the compound, not the solvent
11. The solvent peak should be clearly labeled on the spectrum
12. All peaks should be visible on the spectrum – range should be sufficient to indicate any impurities. Insets are encouraged to show expanded regions. At a minimum, the spectral window should be $-1\text{ ppm to }9\text{ ppm}$ for ^1H NMR and $-10\text{ ppm to }180\text{ ppm}$ for ^{13}C NMR. Ranges should be extended if acid impurities should be indicated.

NOTE: Saving images at resolutions higher than 1200 dpi will not substantially improve the appearance of graphics but will result in large file sizes that inconvenience reviewers, editors, and future readers with long download times. Poor quality spectra can cause delays in evaluating a manuscript.

3.17.3 Primary NMR Data Files

Submission of primary NMR data files (FID files, acquisition data, processing parameters) is encouraged **when the NMR data is critical for the scientific argument**. All original primary NMR data supporting a submission should be retained and provided if requested. When submitting these files one folder should be created for each compound. The folder should be named clearly, using the compound name (if available) and compound identifier, as referenced in the Experimental Section or Supporting Information. Include the FID files, acquisition data and processing parameters for each experiment. Name each spectrum according to the type of nucleus measured: ^1H , ^{13}C , DEPT, COSY, etc. NMR files should be compressed into zip files -- use multiple zip files if necessary. Files must be submitted in their native format.

In a text document, include the name of the manufacturer of the spectrometer used to collect the data, the acquisition software and processing programs used to analyze the data, and the field strength used to measure each nucleus (i.e. 300 MHz ^1H or 50 MHz ^{13}C).

Include a structure file that shows the structure and compound identifier for each provided dataset. MolFile is the recommended format and is strongly preferred.

3.17.4 Crystallographic Information

(See [4.4](#) for the requirements for CIFs.) CIFs should be saved in text-only (plain ASCII) format with .cif as file extension and should not be combined with other types of Supporting Information files. Before being submitted, CIFs should be checked using the free checkCIF data-validation utility on the submission Web site, http://pubs.acs.org/page/4authors/tools/validate_cifs.html. A CIF file should be submitted as 'Supporting Information for Publication' to verify the crystal structure. Any reported syntax errors should be corrected. Manuscripts with uncorrected CIF file syntax errors will be inactivated. (see [2.4](#) for details on inactivation) Any A-level serious alerts should be corrected, or comments inserted into the CIF file regarding their significance. A copy of the final data validation report should be retained in case a reviewer or editor has a question about the data.

3.17.5 Chromatography

HPLC analyses should be performed in two different solvent systems. The stationary phase, solvents (HPLC), detector type, and percentage of total chromatogram integration should be reported; alternatively, a copy of the chromatogram may be included as a figure in the Supporting Information. When flash chromatography is used for product purification, both the support and solvent should be identified.

4. Experimental Data Requirements

If appropriate, a general procedure should be provided as a footnote or in the Supporting Information. Details for specific compounds should be provided as Supporting Information. New procedures should be fully described in detail to ensure reproducibility. New compounds should be characterized by appropriate spectroscopic methods. A criterion of purity must be provided for both new and known compounds whose preparation by a new or improved method is reported (see Section [3.17.1](#) for instructions on reporting experimental data).

4.1 Synthesis Experiments

When a new or improved synthetic method is described, the yields reported in key experimental examples, and yields used for comparison with existing methods, should represent amounts of isolated and purified products, rather than chromatographically or spectroscopically determined yields. Reactant quantities and product yields should be reported in weight or molar units; percentage yields should only be reported for materials of demonstrated purity. When flash chromatography is used for product purification, both the support and solvent should be identified.

4.2 Microwave Experiments

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, and the temperature-time profile. Reporting a wattage rating or power setting is not an acceptable alternative to providing temperature data. Manuscripts describing work done with domestic (kitchen) microwave ovens will not be accepted except for studies where the unit is used for heating reaction mixtures at atmospheric pressure.

4.3 Compound Characterization

Organic Letters 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 all new compounds, evidence adequate to establish both *identity* and *degree of purity* (homogeneity) should be provided (see [4.3.2](#) and [4.3.3](#) ‘Identity’ and ‘Purity’). Purity documentation must be provided for known compounds whose preparation by a new or improved method is reported (see [4.3.3](#)). In addition, for noncommercial, known compounds used as starting materials, the method of preparation and the literature data used to confirm the materials’ identity should be cited. Listings of IR absorptions and NMR resonances for known compounds should be presented only if they do not duplicate previously published data.

Submission of a Compound Characterization Checklist, developed by our sister publication, *The Journal of Organic Chemistry* is recommended *but not required*. Many reviewers and editors find that this compilation of physical, analytical, and spectral data greatly facilitates evaluation of manuscripts. A copy of this Checklist is included at the end of these guidelines and is also available at <http://pubs.acs.org/page/orlef7/submission/ccc.html>.

4.3.1 Guidelines for Specific Compound Classes

Combinatorial libraries containing more than 20 compounds: complete characterization data must be provided for at least 20 diverse members.

Natural products whose structures are being proposed or revised: sufficient data should be provided to definitively establish molecular composition. Suggested analyses include: ¹H/¹³C NMR, HRMS, and IR spectra (with data); 2D ¹H COSY, 2D ¹H/¹³C HMQC, and 1D DEPT spectra as well as long-range ¹H COSY spectra and NOESY and/or NOE spectra (where NOE data is being used to assign a structure). An X-ray crystal structure can also be employed to establish the structure assignment. Specific optical rotations, [α]_D values, should be reported for isolated natural products and enantiopure compounds.

Configurational Isomer Mixtures: For reporting the compositions, enantiomer or diastereomer ratios are preferred over enantiomeric or diastereomeric excess values.

Non-racemic chiral substances: data to permit correlation of absolute configuration should be provided, preferably including [α]_D values.

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 that establish the molecular weight

4.3.2 Identity

(1) *Spectra/Spectral Data.* Copies of ¹H and ¹³C NMR spectra should be provided for key transformations and final products. (see Section [3.17.2](#) for requirements for presenting spectra) 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.

While we recognize that *Organic Letters* comprises preliminary reports, we are committed to providing the organic community with the most reliable and well-documented methods in the chemical literature, therefore these key spectra are requested rather than simply a list of resonances. Copies of spectra should also be included where structure assignments of complex molecules depend heavily on NMR interpretation (see [3.17.2](#) for requirements for presenting spectra).

For other new compounds, a listing of ^1H and ^{13}C resonances and important IR adsorptions should be given. HPLC/LCMS can be substituted for biochemistry papers where the main focus is not on compound synthesis. ^{13}C NMR peak shifts should be rounded to the nearest 0.1 ppm unless greater precision is needed to distinguish closely spaced peaks. Hydrogen multiplicity (C, CH, CH₂, CH₃) information obtained from routine DEPT spectra should be included. If detailed peak assignments are made, the type of NOESY or COSY methods used to establish atom connectivities and spatial relationships should be identified in the Supporting Information.

(2) *HRMS/elemental analysis*. To support the molecular formula assignment, HRMS data accurate within 5 ppm, or combustion elemental analysis data accurate within 0.4%, should be reported for new compounds. NOTE: in certain cases, a crystal structure may be an acceptable substitute for HRMS/elemental analysis. A CIF file should be submitted to verify the crystal structure (see Sections [3.17.1](#) and [4.4](#) for information on submitting CIF files

(3) *Melting point*. A melting point *range* should be reported for all crystalline compounds. Melting points of noncrystalline amorphous compounds should not be reported.

(4) *Specific rotations*. Specific rotations based on the equation $[\alpha] = (100 \cdot \alpha) / (l \cdot c)$ should be reported as unitless numbers as in the following example: $[\alpha]^{20}_{\text{D}} -25.4$ (c 1.93, CHCl₃), where the concentration c is in g/100 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.

4.3.3 Purity

Evidence for documenting compound purity should include one or more of the following:

(1) A standard 1D proton-decoupled ^{13}C NMR spectrum or a well-resolved high field ^1H NMR spectrum showing at most only trace peaks not

attributable to the assigned structure. Range of spectra should be sufficient to indicate any impurities. (see [3.17.2](#) for requirements for presenting spectra)

(2) Combustion elemental analytical values for carbon and hydrogen (and nitrogen, if present) agreeing with calculated values within 0.4%.

(3) 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. HPLC analyses should be performed in two diverse systems. The stationary phase, solvents (HPLC), detector type, and percentage of total chromatogram integration should be reported; alternatively, a copy of the chromatogram may be included as a figure in the Supporting Information.

(4) Electrophoretic analytical data obtained under conditions that permit observing impurities present at the 5% level.

The types 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 a good choice for the product of an isomerization or rearrangement reaction; a "clean" NMR spectrum would need to be supplemented with other evidence when a reasonably likely impurity is NMR silent (e.g., an inorganic salt). HRMS data may be used to support a molecular formula assignment *but cannot be used as a criterion of purity*.

4.4 Crystal Data

Authors are encouraged to submit crystallographic information in the Crystallographic Information File (CIF) format, *even if the data have been deposited with a crystallographic database*. One printed table of Structure Factors should be retained by the author and supplied, if requested, for review purposes only; *do not submit it as Supporting Information* (see [3.17.4](#) for information on submitting CIF files).

4.5 Computational Data

When computational results are included in a manuscript, complete details of computational methods and results, reported in sufficient detail to allow other researchers to repeat the computations, should be included either within the paper or in the Supporting Information. The level of theory, basis set, and relevant input parameters should be identified along with the specific program used, including information sufficient for the reader to use the program if desired. The data should

include Z-matrices or Cartesian coordinates, grid size (for DFT calculations) and computed total energies of target or optimized structures. Where applicable, the number of imaginary frequencies should be reported to identify stable structures and transition states. Graphics of computationally derived models that are not vital to the discussion should be placed in the Supporting Information.

4.6 Hazards

Any unusual hazards in the chemicals, equipment, or procedures used in an investigation should be clearly identified in a numbered footnote in the manuscript.

5. Artwork

Artwork may be categorized into structure blocks, equations (numbered reactions), schemes, and figures. Equations, schemes, and figures should be numbered using Arabic numbers, with a separate numbering sequence for each category. Schemes may have titles and footnotes; figures should have captions. Structures should be numbered with boldface Arabic numbers. Remove all color from graphics, except for those graphics that you would like to have considered for publication in color (see [5.3](#) for details).

The quality of the illustrations in the journal depends on the quality of the originals. Artwork should be provided at the size it will be published in the Journal. Chemical structure graphics and figures cannot be modified or enhanced by the journal production staff. Any changes to the artwork (including size changes) must be made in the drawing program that was used to create the artwork, and the revised artwork reimported into the manuscript. The artwork should follow the first mention in the text and should be designed to use space efficiently so that it can be integrated into the Letter where it is mentioned. One-column artwork is strongly recommended. Artwork that straddles two columns should be placed at the top of a page in the template. Structure sizes should be consistent throughout all schemes and figures. Lettering and lines should be of uniform density. Arial or Helvetica font should be used for text; the size should be at least 5.0 points. Lines should be no thinner than 1.0 point. NOTE: Do not provide additional copies of artwork as Supporting Information, Review-Only Material, or with file designation ‘Graphic for Manuscript’.

5.1 Preparation

All artwork should be produced with a drawing program such as ChemDraw and constructed in keeping with the journal column widths: single column, 3.3 in. (8.5 cm); double column, 7.0 in. (17.8 cm). Arial or Helvetica font should be used for all text in schemes, figures, and structure blocks. Artwork should be provided at the proper size for publication. Further details concerning drawing settings are given in ‘Working with Graphics’ on the ‘Manuscript Submission and Peer Review

in ACS Paragon Plus' page:

http://pubs.acs.org/page/4authors/submission/graphics_prep.html.

5.2 ChemDraw

For ChemDraw users, two ChemDraw Style Sheet files (for 1 and 2 column graphics) are available from the Organic Letters web page containing the manuscript templates (see Submission & Review tab, Info for Authors) (<http://pubs.acs.org/OrgLett>). Use of these files will ensure that your graphics are sized properly. Also, recent versions of ChemDraw provide the recommended structure drawing settings as a formatting option: "ACS Document 1996". Authors not using ChemDraw and those using an early version of ChemDraw without the pre-set formatting should refer to 'Working with Graphics' on the 'Manuscript Submission and Peer Review in ACS Paragon Plus' page: <http://paragonplus.acs.org>. Graphics should have the following minimum resolution:

Black and white line art	1200 dpi
Grayscale art	600 dpi
Color art (RGB)	300 dpi

NOTE: Saving images at resolutions higher than 1200 dpi will not substantially improve the appearance of graphics but will result in large file sizes that inconvenience reviewers, editors, and future readers with long download times.

The RGB and resolution requirements are essential for producing high-quality graphics within 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.

5.3 Color

Color reproduction, where appropriate, will be provided at no cost to the author. Where possible, red is preferred for better visibility. Color in graphs is discouraged.

6. Revisions

The Editors' acceptance of a manuscript for publication is contingent on the author's submitting, within a reasonable time, a revised manuscript appropriately addressing reviewer and Editor concerns. If the revised manuscript is not submitted within the time requested, and no specific arrangements for completion are made with the Editor, the manuscript will be inactivated. In preparing the final revision of an accepted manuscript, the author should address the comments provided by

the Editor or reviewers. **These comments should be addressed not only in the response letter but also within the body of the revised manuscript itself.**

Changes to the manuscript, whether or not made in response to those comments, as well as any change to the title or to the author list should be described in the 'Response to Decision Letter' section at the revision submission site. A revision cover letter can also be submitted but is not required.

7. Proofs

The corresponding author of an accepted manuscript will receive e-mail notification and complete instructions when page proofs are available for review 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.

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12. Updated Instructions

As additional features become available, these instructions will be updated on the *Organic Letters* homepage at <http://pubs.acs.org/OrgLett>.

13. Standard Abbreviations and Acronyms

α	observed optical rotation in degrees	DCC	<i>N,N'</i> -dicyclohexylcarbodiimide
$[\alpha]$	specific rotation [expressed without units; the units, (deg·mL)/(g·dm), are understood]	DCE	1,2-dichloroethane
Å	angstrom(s)	DDQ	2,3-dichloro-5,6-dicyano-1,4-benzoquinone
Ac	acetyl	DEAD	diethyl azodicarboxylate
acac	acetylacetonate	DEPT	distortionless enhancement by polarization transfer
ADP	adenosine 5'-diphosphate	DFT	density functional theory
AIBN	2,2'-azobisisobutyronitrile	DIBALH	diisobutylaluminum hydride
AM1	Austin model 1	DMA	dimethylacetamide
AMP	adenosine 5'-monophosphate	DMAP	4-(<i>N,N</i> -dimethylamino)pyridine
Anal.	combustion elemental analysis	DMDO	dimethyldioxirane
anhyd	anhydrous	DME	1,2-dimethoxyethane
AO	atomic orbital	DMF	dimethylformamide
aq	aqueous	DMPU	1,3-dimethyl-3,4,5,6-tetrahydro-2(1 <i>H</i>)-pyrimidinone
Ar	aryl	DMSO	dimethyl sulfoxide
atm	atmosphere(s)	DMT	4,4'-dimethoxytrityl (4,4'-dimethoxyltriphenylmethyl)
ATP	adenosine 5'-triphosphate	DNA	deoxyribonucleic acid
ATPase	adenosinetriphosphatase	DPS	<i>tert</i> -butyldiphenylsilyl
av	average	dr	diastereomeric ratio
9-BBN	9-borabicyclo[3.3.1]nonyl	DTT	dithiothreitol
9-BBN-H	9-borabicyclo[3.3.1]nonane	E1	unimolecular elimination
Bn, Bzl	benzyl	E2	bimolecular elimination
bpy	2,2'-bipyridyl	ED50	dose effective in 50% of test subjects
BOC, Boc	<i>tert</i> -butoxycarbonyl	EDTA	ethylenediaminetetraacetic acid
bp	boiling point, base pair	EI	electron impact
br	broad (spectral)	EPR	electron paramagnetic resonance

Bu, <i>n</i> -Bu	normal (primary) butyl	eq	equation
<i>s</i> -Bu	<i>sec</i> -butyl	equiv	equivalent
<i>t</i> -Bu	<i>tert</i> -butyl	er	enantiomeric ratio
Bz	benzoyl (not benzyl)	ESI	electrospray ionization
B3LYP	3-parameter hybrid Becke exchange/ Lee–Yang–Parr correlation functional	Et	ethyl
°C	degrees Celsius	FAB	fast atom bombardment
calcd	calculated	FD	field desorption
cAMP	adenosine cyclic 3',5'-phosphate	FID	flame ionization detector; free induction decay
CAN	ceric ammonium nitrate	Fmoc	9-fluorenylmethoxycarbonyl
CASSCF	complete active space self-consistent field	FT	Fourier transform
CASPT2	complete active space with second-order perturbation theory	g	gram(s); prefix to NMR abbreviation denoting gradient-selected (e.g. gCOSY, gHMQC)
Cat.	catalytic	GC	gas chromatography
CBZ, Cbz	benzyloxycarbonyl (preferred over the abbreviation Z)	GTP	guanosine 5'-triphosphate
CC	coupled cluster	h	hour(s)
CD	circular dichroism	HF	Hartree–Fock
cDNA	complementary deoxyribonucleic acid	HMBC	heteronuclear multiple bond correlation
<i>c</i> -Hex, <i>c</i> -C ₆ H ₁₁	cyclohexyl	HMPA	hexamethylphosphoric triamide (hexamethylphosphoramide)
CI	chemical ionization; configuration interaction	HMQC	heteronuclear multiple quantum correlation
CIF	crystallographic information file	HOMO	highest occupied molecular orbital
CIDNP	chemically induced dynamic nuclear polarization	HPLC	high-performance liquid chromatography
cm	centimeter(s)	HRMS	high-resolution mass spectrometry
cm ⁻¹	wavenumber(s)	HSQC	heteronuclear single quantum correlation
cod	1,5-cyclooctadiene	Hz	hertz
compd	compound	ICR	ion cyclotron resonance
concd	concentrated	INDO	intermediate neglect of

concn	concentration	IP	differential overlap
COSY	correlation spectroscopy	IR	ionization potential
cot	1,3,5,7-cyclooctatetraene	<i>J</i>	infrared
Cp	cyclopentadienyl	<i>k</i>	coupling constant (in NMR spectrometry)
<i>m</i> -CPBA	<i>meta</i> -chloroperoxybenzoic acid	K	kilo
CV	cyclic voltammetry	L	kelvin(s) (absolute temperature)
δ	chemical shift in parts per million downfield from tetramethylsilane	LAH	liter(s)
d	day(s); doublet (spectral); deci	LCAO	lithium aluminum hydride
<i>d</i>	density	LD ₅₀	linear combination of atomic orbitals
DABCO	1,4-diazabicyclo[2.2.2]octane	LDA	dose that is lethal in 50% of test subjects
dansyl	5-(dimethylamino)-1-naphthalenesulfonyl	LFER	lithium diisopropylamide; local density approximation
DBN	1,5-diazabicyclo[4.3.0]non-5-ene	LHMDS	linear free energy relationship
DBU	1,8-diazabicyclo[5.4.0]undec-7-ene	lit.	lithium hexamethyldisilazane, lithium bis(trimethylsilyl)amide
LTMP	lithium 2,2,6,6-tetramethylpiperidide	PT	literature value (abbreviation used with period)
LUMO	lowest unoccupied molecular orbital	PTC	perturbation theory
μ	micro	py	phase-transfer catalysis
m	multiplet (spectral); meter(s); milli	q	pyridine
M	molar (moles per liter); mega	QSAR	quartet (spectral)
M ⁺	parent molecular ion	RCM	quantitative structure–activity relationship
MALDI	matrix-assisted laser desorption ionization	redox	ring-closure metathesis
max	maximum	rel	reduction–oxidation
MCD	magnetic circular dichroism	<i>R_f</i>	relative retention factor (in chromatography)

MCR	multicomponent reaction	RHF	restricted Hartree–Fock
MCSCF	multi-configuration self-consistent field	ROESY	rotating frame Overhauser effect spectroscopy
MD	molecular dynamics	ROMP	ring-opening metathesis polymerization
Me	methyl	rRNA	ribosomal ribonucleic acid
MEM	(2-methoxyethoxy)methyl	rt	room temperature
Mes	2,4,6-trimethylphenyl (mesityl) [not methylsulfonyl (mesyl)]	s	singlet (spectral); second(s)
MHz	megahertz	SAR	structure–activity relationship
min	minute(s); minimum	SCF	self-consistent field
mM	millimolar (millimoles per liter)	SEM	scanning electron microscopy
MO	molecular orbital	S _N 1	unimolecular nucleophilic substitution
mol	mole(s); molecular (as in mol wt)	S _N 2	bimolecular nucleophilic substitution
MOM	methoxymethyl	S _N '	nucleophilic substitution with allylic rearrangement
mp	melting point	SOMO	single-occupied molecular orbital
MP	Møller–Plesset perturbation theory	t	triplet (spectral)
MRCI	multi-reference configuration interaction	<i>T</i>	time; temperature in units of degrees Celsius (°C)
mRNA	messenger ribonucleic acid	<i>T</i>	absolute temperature in units of kelvins (K)
Ms	methylsulfonyl (mesyl)	TBAB	tetrabutylammonium bromide
MS	mass spectrometry	TBAC	tetrabutylammonium chloride
MTBE	methyl <i>tert</i> -butyl ether	TBAF	tetrabutylammonium fluoride
MW, mol wt	molecular weight	TBS	<i>tert</i> -butyldimethylsilyl
<i>m/z</i>	mass-to-charge ratio (not <i>m/e</i>)	TBHP	<i>tert</i> -butyl hydroperoxide
N	normal (equivalents per liter)	TCA	trichloroacetic acid
NAD ⁺	nicotinamide adenine dinucleotide	TCNE	tetracyanoethylene
NADH	reduced NAD	TDDFT	time-dependent density functional theory
NBO	natural bond orbital	TEAB	tetraethylammonium bromide

NBS	<i>N</i> -bromosuccinimide	Temp	temperature
NCS	<i>N</i> -chlorosuccinimide	Tf	trifluoromethanesulfonyl (triflyl)
NICS	nucleus-independent chemical shift	TFA	trifluoroacetic acid
nm	nanometer(s)	TFAA	trifluoroacetic anhydride
NMO	<i>N</i> -methylmorpholine- <i>N</i> - oxide	THF	tetrahydrofuran
NMP	<i>N</i> -methylpyrrolidone	SET	single electron transfer
NMR	nuclear magnetic resonance	THP	tetrahydropyran-2-yl
NOE	nuclear Overhauser effect	TIPS	triisopropylsilyl
NOESY	nuclear Overhauser effect spectroscopy	TLC	thin-layer chromatography
NRT	natural resonance theory	TMAI	tetramethylammonium iodide
Nu	nucleophile	TMEDA	<i>N,N,N',N'</i> -tetramethyl-1,2- ethylenediamine
obsd	observed	TMS	trimethylsilyl; tetramethylsilane
OD	optical density	TOF	time-of-flight
ORD	optical rotary dispersion	Tr	triphenylmethyl (trityl)
PCC	pyridinium chlorochromate	tRNA	transfer ribonucleic acid
PDC	pyridinium dichromate	<i>t_R</i>	retention time (in chromatography)
PES	photoelectron spectroscopy	Ts	<i>p</i> -toluenesulfonyl (tosyl)
Ph	phenyl	TS	transition state
piv	pivaloyl	UHF	unrestricted Hartree–Fock
pm	picometer(s)	UV	ultraviolet
PM3	parametric method 3	VCD	vibrational circular dichroism
PMB	<i>p</i> -methoxybenzyl	vis	visible
PPA	poly(phosphoric acid)	vol	volume
ppm	part(s) per million	v/v	volume per unit volume (volume-to-volume ratio)
PPTS	pyridinium <i>p</i> - toluenesulfonate	wt	weight
Pr	propyl	w/w	weight per unit weight (weight-to-weight ratio)
<i>i</i> -Pr	isopropyl	ZINDO	Zerner parameterization of intermediate neglect of differential overlap

14. Compound Characterization Checklist

RECOMMENDED COMPOUND CHARACTERIZATION CHECKLIST

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FOR ORGANIC LETTERS

Corresponding Author

Manuscript Title

NOTE: THE CHECKLIST IS RECOMMENDED BUT IS NOT REQUIRED

1. Please copy this Checklist form and complete the form by hand (**An Excel version is available at the web submission site.**).
2. Enter the name of the corresponding author and the title of the manuscript above. If known, enter the manuscript number next to "OL".
3. In the left-most column, enter the identifying numbers (or table-entry numbers) of the compounds or structures for which data are reported.

List them in the sequence in which they appear in the manuscript (and in the supporting information, if there is any). For each compound, type a single "X" in either the "New compound" column or the "Known compound" 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 the unlabeled columns for data types not listed. It is not expected that all or most of the columns be marked, only those needed to establish compound identity and purity.

5. Please scan the completed Checklist, save the scanned image(s) in JPEG, GIF, or PDF format, and upload with your manuscript submission.

Compound, entry number	IDENTITY		PURITY	COMPUTATIONAL DATA in SI*		Supporting Information	
	New compound	Known compound Melting point range IR UV-vis ¹ H NMR ¹³ C NMR Other NMR [type:] MS HRMS Optical rotation/ORD/CD X-ray [ORTEP and CIF in SI*] Enantiomeric/diastereomeric ratio Copy of ¹ H/ ¹³ C NMR spectrum in SI* Quant: GC, HPLC, or electrophoresis Elemental analysis Cartesian coordinates or Z-matrix # of imaginary frequencies Total energy * SI =					

