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SCOPE OF THE JOURNAL

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

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

(a) Single or multistep synthetic methods manuscripts and total synthesis manuscripts are expected to demonstrate strategies, transformations, or shortened routes to target structures that show conceptual novelty, not merely the extension of previously reported chemistry to a different class of reaction substrates, reagents, or catalysts.

(b) Manuscripts focusing on mechanistic studies (experimental or theoretical) should show methodological advances or provide novel insight into the course of chemical reactions, rather than only confirming previously established mechanisms.

(c) Natural products isolation and identification studies should report unusual skeletal features, improvements in methods for structural determination, or insights into biosynthetic pathways.

(d) Manuscripts with elements of biological study, analytical chemistry, functional molecules and systems, or materials science should demonstrate novelty in those aspects associated with the organic chemistry portion of the work being reported.

MANUSCRIPT TYPES

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

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

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

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

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

**ACS PUBLISHING CENTER**

While this document will provide basic information on how to prepare and submit the manuscript as well as other critical information about publishing, we also encourage authors to visit the ACS Publishing Center for additional information on everything that is needed to prepare (and review) manuscripts for ACS journals, such as

- [Mastering the Art of Scientific Publication](#) which shares editor tips about a variety of topics including making your paper scientifically effective, preparing excellent graphics, and writing cover letters.
- Resources on [how to prepare and submit a manuscript](#) to ACS Paragon Plus, ACS Publications’ manuscript submission and peer review environment.
- [Sharing your research](#) with the public through ACS Publications open access program

**MANUSCRIPT PREPARATION**

**Review Ready Submission**

All ACS journals have simplified their formatting requirements in favor of a streamlined and standardized review-ready format for an initial manuscript submission. Read more about the requirements and the benefits these serves authors and reviewers [here](#). Manuscripts submitted for initial consideration must adhere to these standards:

- Submissions must be complete with clearly identified standard sections used to report original research, free of annotations or highlights, and include all numbered and labeled components.
- Figures, charts, tables, schemes, and equations should be embedded in the text at the point of relevance. Separate graphics can be supplied later at revision, if necessary.
- A two-column manuscript template is available and can be used for manuscripts submitted to any ACS journal. Templates are not required but may be useful to approximate how an article will compose. For manuscripts with word count limits, authors are not required to fit content into a page limit based on the template.
- References can be provided in any style, but they must be complete, including titles.
• Supporting Information should be submitted as a separate file(s).
• Author names and affiliations on the manuscript must match what is entered into ACS.

**Document Templates and Format**
The templates facilitate the peer review process by allowing authors to place artwork and tables close to the point where they are discussed within the text. Learn more about document templates here.

General information on the preparation of manuscripts may also be found in The ACS Style Guide.

**Acceptable Software, File Designations, and TeX/LaTeX**
See the list of Acceptable Software and appropriate File Designations to be sure your file types are compatible with ACS Paragon Plus. Information for manuscripts generated from TeX/LaTeX is also available.

**Cover Letter**
A cover letter must accompany every manuscript submission. During the submission process, you may type it or paste it into the submission system, or you may attach it as a file.

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

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

Claims of priority, originality, convenience, effectiveness, or value should be avoided or used with great restraint. For example, the words “convenient”, “efficient”, “elegant”, “expedient”, “facile”, “first”, "new", "novel", "practical", "simple", “unique”, “unprecedented”, and "versatile" should not be used. In addition, editors may ask authors to moderate or remove what they judge to be excessive use of subjective evaluative language elsewhere in the manuscript.

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

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

**Abbreviations, Symbols, Units, Compound Names.** Authors are encouraged to use abbreviations and acronyms in the text to conserve space. A checklist is available to assist with common abbreviations and formatting conventions for tables and schemes. 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. Full systematic names of compounds (see the ACS Style Guide for guidance) should be included in the Experimental Section on first mention and for brevity assigned a molecule number for reference throughout the article. In the Introduction, Results and Discussion, and Conclusions, authors should use their judgement on common usage of compound names or use molecule numbers in lieu of full systematic names.

**Abstract.** The abstract for an Article or Note should briefly state the purpose of the research, the principal results, and the major conclusions. A well-written abstract can attract the attention of potential readers and increase the likelihood that the published paper will be cited by other researchers. Summaries of numerical results should be quantitative (for example, "in yields of 65 to 90%" rather than "in good to excellent yields").

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

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

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

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

**Experimental Section.** For Notes and Articles, every manuscript reporting the results of experimental work must include an experimental section, and all experimental procedures, compound characterization data, and any associated literature citations must appear in the manuscript’s experimental section. This section should describe experimental methods in sufficient detail to permit repetition of the work by others. These procedures and data listings should not be duplicated in the supporting information. 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. A General Experimental Methods paragraph may be optionally provided to document procedures (such as purification methods, solvent
removal, and spectroscopic and chromatographic analyses) that are common to most of the individual procedures, and should be placed at the beginning of the experimental section (see Data Requirements for more details).

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

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

**Supporting Information**
This information is provided to the reviewers during the peer-review process (for Review Only) and is available to readers of the published work (for Publication). Supporting Information must be submitted at the same time as the manuscript. See the list of Acceptable Software by File Designation and confirm that your Supporting Information is viewable.

If the manuscript is accompanied by any supporting information files for publication, these files will be made available free of charge to readers. A brief description of each file is required, and the paragraph and descriptions should be placed at the end of the manuscript before the list of references. The appropriate format is as follows:

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

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

**Data Requirements**
For Notes and Articles, every manuscript reporting the results of experimental work must include an experimental section, and all experimental procedures, compound characterization data, and any associated literature citations must appear in the manuscript’s experimental section. This section should describe experimental methods in sufficient detail to permit repetition of the work by others. These procedures and data listings should not be duplicated in the Supporting Information. The section on “Specialized Data” should be consulted for guidance on reporting synthetic experimental, compound characterization, spectroscopic, crystallographic, computational, and bioassay data in the Experimental Section and Supporting Information.
General Experimental Methods. A General Experimental Methods paragraph may be optionally provided to document procedures (such as purification methods, solvent removal, and spectroscopic and chromatographic analyses) that are common to most of the individual procedures, and should be placed at the beginning of the experimental section.

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

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

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

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

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

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

All reported yields should represent weighed amounts of isolated and purified products and must be reported in the experimental section as both weights and percentages. When a series of related compounds has been prepared using substantially the same procedure, it is usually sufficient to present a single representative example. If instead a general synthesis procedure reporting only relative molar quantities (as equivalents) is presented, the relative solvent volume also needs to be reported (as the molarity of the limiting reactant or reagent in the reaction mixture). If the several examples were not all conducted at the same molar scale, the paragraphs describing the individual products should include, along with the yields, the weights and molar amounts of the limiting reactants, for example, “yield 177 mg (78%) from 198 mg (0.66 mmol) of 3d.”

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

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

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

The Editors encourage authors to emphasize any unexpected, new, and/or significant hazards or risks associated with the reported work, including the use of toxic and/or environmentally persistent reagents and solvents, and provide a rationale on choice of these reagents and solvents. JOC further encourages authors to consider the Principles of Green Chemistry in carrying out their research and consider reporting metrics such as atom economy, mass efficiency, E-factor, or others. For more information, please consult Research Tools provided by the ACS Green Chemistry Institute.

Compound Characterization Data

JOC upholds a high standard for compound characterization to ensure that compounds being added to the chemical literature have been correctly identified and can be synthesized in known yield and purity. For new compounds, evidence adequate to establish both identity and degree of purity (homogeneity) must be provided. Purity documentation must also be provided for known compounds whose preparation by a new or modified literature method is reported. JOC requires that purity be documented compound-by-compound, with copies of spectra or chromatograms, elemental analysis, or quantitative NMR or chromatographic integration data. For combinatorial libraries containing more than 20 new compounds, complete characterization data must be provided for at least 20 diverse members of each structural type. Full characterization is not required for new compounds prepared solely as derivatives for analytical purposes (for example, Mosher esters prepared for assigning absolute configuration).
Authors are responsible for retaining their original data or having available original data from collaborators or from contractors who perform analyses on their behalf. Authors may be asked to provide copies of spectra or analytical reports if an editor or reviewer raises a question about reported results.

A completed Compound Characterization Checklist must be provided when reporting new compounds or when reporting known compounds that have been prepared by new or modified methods. Known compounds that have been synthesized by literature methods or obtained from commercial sources should not be listed, but appropriate references or sources should be cited. The Checklist will help editors and reviewers assess the thoroughness of the characterization of compounds and the reporting of computational results.

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

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

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

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

All compound preparation procedures and characterization data should be included in the manuscript 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, except that NMR and accurate mass (HRMS) data should be reported as discussed below. For compounds that have been prepared by more than one method, the description in the experimental section and the purity documentation (usually a proton NMR spectrum in the Supporting Information) should clearly identify which method provided the sample whose yield and purity are documented.

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

NMR (consult ACS NMR Guidelines for additional details). Proton and carbon NMR resonances should be listed for each new compound, with the normal full range of chemical shifts displayed (usually 0–10 ppm for proton; 0–200 ppm for carbon); the solvent and instrument frequency should be identified. The use of broadband decoupling should be indicated with braces, for example $^{13}\text{C}\{^1\text{H}\}$ for proton-decoupled carbon data. Proton NMR shifts, reported to 0.01 ppm precision, should be accompanied by an abbreviation for any multiplet structure, the number of atoms represented by the peak or multiplet, and coupling constants where applicable. Carbon NMR peak shifts should be rounded off to the nearest 0.1 ppm except when greater precision is needed to distinguish closely spaced peaks. Information about numbers of attached hydrogen atoms (reported as C, CH, CH$_2$, CH$_3$) from DEPT, DEPTQ, PENDANT, or 2D spectra may be included with the carbon peak shifts. For compounds with carbon-bonded fluorine atoms, the carbon peak multiplicity (d, t, q) and coupling in Hz should be reported. Detailed peak assignments (including "ArH" for aromatic protons and "C=O" for carbonyl carbons) should not be reported in the experimental section unless one or more 2D methods have been used to establish atom connectivities and spatial relationships, and the type(s) of 2D methods are identified in a General Experimental Methods paragraph (section 2.1.9) or in the individual compound data listings. Authors using software for automated data analysis are reminded to check numerical data (including proton counts and coupling constants) before including them in the manuscript.

For products isolated as inseparable isomer mixtures, if the NMR absorptions can be attributed to individual isomers, the NMR chemical shift data for those isomers should be reported in two or more separate lists, one for each isomer, instead of as a single list. For proton NMR data, the integrals in each isomer's list should be reported in whole numbers of protons.

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

One of the purposes of including copies of NMR spectra in the supporting information is to qualitatively demonstrate the purity of the materials obtained when the reported reaction, isolation, and purification methods are used. It is not acceptable to use peak-editing software or other means to suppress or obscure peaks arising from impurities (including byproducts, 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.

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. The FID data should be mentioned in the manuscript file supporting information availability statement. 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 (high-resolution mass spectrometry [HRMS] or "exact mass") data should be reported to support the molecular formula assignment. The data should be reported in *ACS Style Guide* format and should include the molecular formulas on which the theoretical (Calcd) values are based.

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

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

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

The *ACS Style Guide* format for reporting elemental analysis data is: Anal. Calcd for C_{13}H_{17}NO_3: C, 66.36; H, 7.28; N, 5.95. Found: C, 66.55; H, 7.01; N, 6.22. Elemental analysis Found values for carbon, hydrogen, and nitrogen should be within 0.4% of the Calcd values for the proposed formula. The need to include fractional molecules of solvent or water in the molecular formula to improve the fit of the data usually reflects incomplete purification of the sample. In such cases, either a portion of the product should be repurified and reanalyzed, or HRMS data should be obtained. If any of the reported formulas include solvent or water, independent evidence for its presence needs to be reported immediately following the Found values.

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

A single-crystal X-ray diffraction structure 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 \([\alpha] = \frac{(100\cdot\alpha)}{(l\cdot c)}\) should be reported as unitless numbers as in the following example: \([\alpha]_D^{20} = 25 \pm 0.25 \text{ (c 1.9, CHCl}_3\)), where the concentration \(c\) is in g/100 mL and the path length \(l\) is in decimeters. The units of the specific rotation, \((\text{deg} \cdot \text{mL})/(\text{g} \cdot \text{dm})\), are implicit and are not included with the reported value.

**Physical State and Melting Point.** The description of new compounds should include a statement of whether the isolated material is a crystalline solid, an amorphous solid, a gum, or a liquid. The color should be reported if it is not colorless or white. A melting point range should be reported for every new crystalline solid product. Melting point ranges may be reported to document the purity of known, but not new, synthesis products (see below). Authors are encouraged to report melting point ranges for recrystallized samples of known compounds that were previously reported only in noncrystalline (and presumably less pure) form.

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

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

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- Combustion elemental analytical values for carbon and hydrogen (and nitrogen, if present) agreeing with calculated values within 0.4%.
• Quantitative NMR data using an internal standard and based on peak area ratios determined under conditions that assure complete relaxation.

• Quantitative gas chromatographic analytical data for distilled or vacuum-transferred samples, or quantitative HPLC analytical data for materials isolated by column chromatography or separation from a solid support. The stationary phase, solvent (HPLC), detector type, and percentage of total chromatogram integration represented by the product peak should be reported. Alternatively, a copy of the chromatogram may be included in the supporting information.

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

• For known solid compounds, a narrow melting point range that is in close agreement with a cited literature value.

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

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

**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, should be included. Spectra used as adjuncts to the characterization of compounds should be included in the supporting information.

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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.

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

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- Color art 300 dpi

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Graphics must fit a one- or two-column format. Single-column graphics can be sized up to 240 points wide (3.33 in.) and double-column graphics must be sized between 300 and 504 points (4.167 in. and 7
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